A Genetic Algorithm Approach to Guiding the Evolution of Self-Organised Nanostructured Systems

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Condensed Matter and Materials Physics

20th April, University of Exeter

The University of Nottingham

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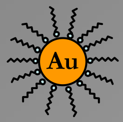
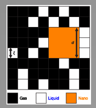
CMMP06

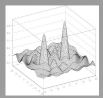
Overview



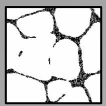
- Physical background



- Nanoparticle simulation details



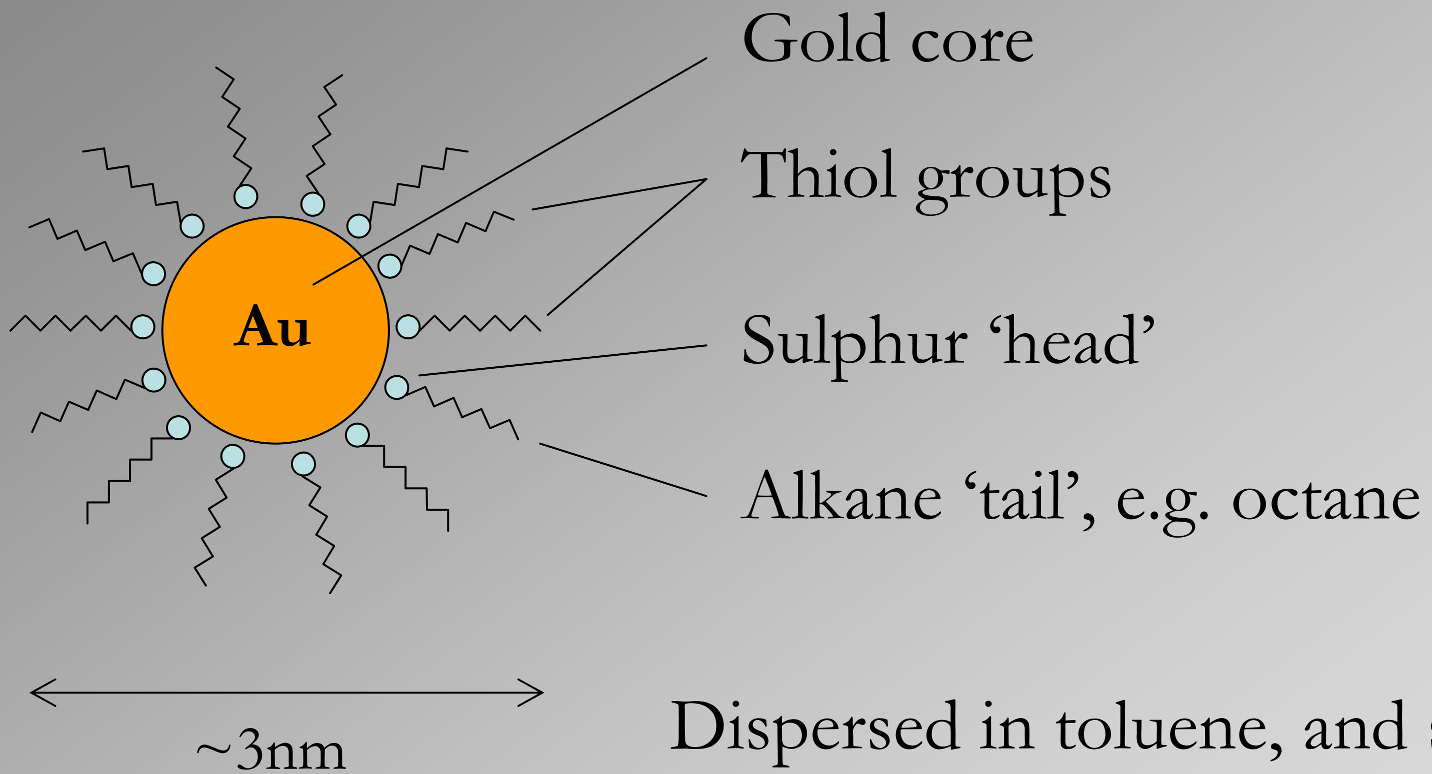
- A brief overview of Genetic Algorithms



- Results from initial trials

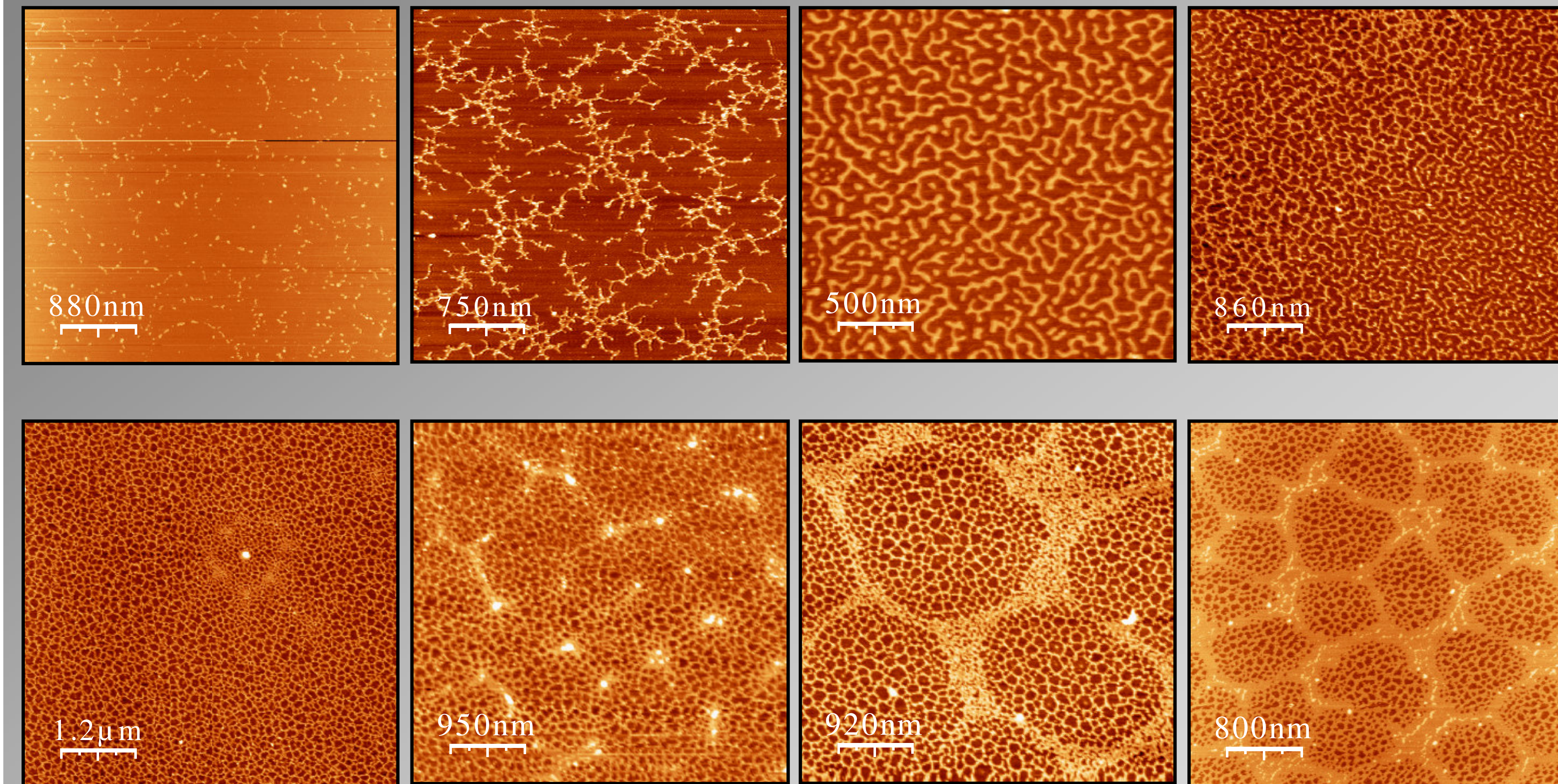
- Conclusions & further work

Thiol-passivated Au nanoparticles



Dispersed in toluene, and spin cast onto native-oxide-terminated silicon

Au nanoparticles: Morphology



AFM images taken by Matthew O. Blunt, Nottingham

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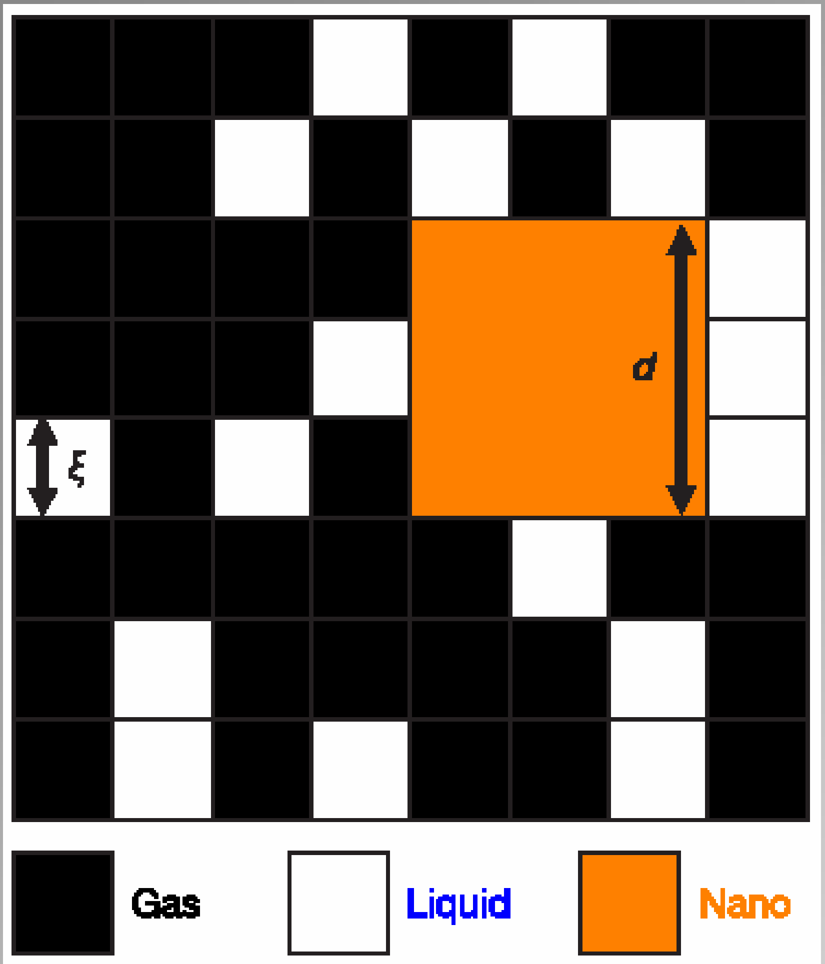
Nanoparticle Simulations



Solvent is represented as a two-dimensional lattice gas

Each lattice site represents 1nm^2

Nanoparticles are square, and occupy nine lattice sites

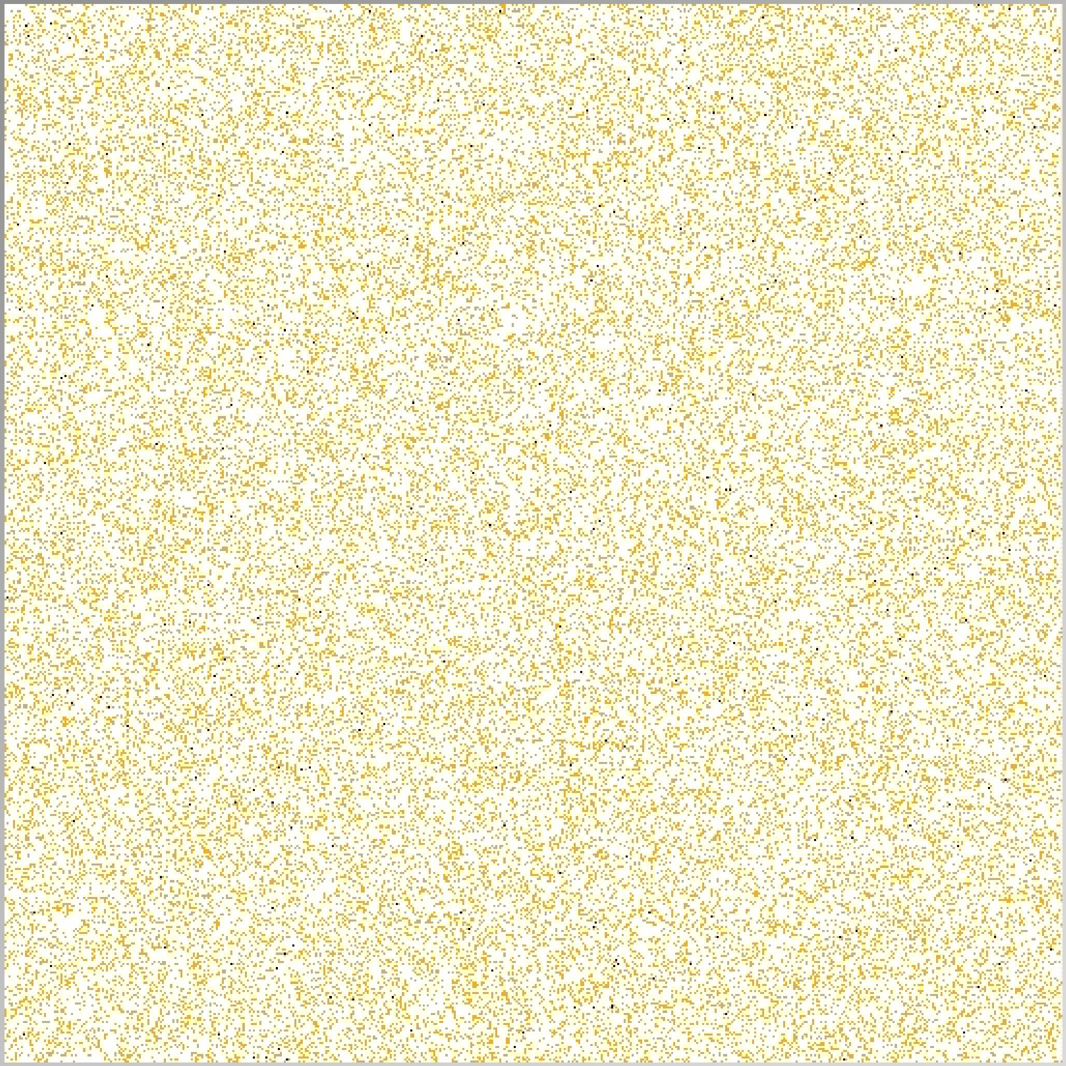
Based on the simulations of Rabani et al. (*Nature* **2003**, *426*, 271-274). Includes modifications to include next-nearest neighbours to remove anisotropy.

Nanoparticle Simulations

- The simulation proceeds by the Metropolis algorithm:
  - Each solvent cell is examined and an attempt is made to convert from liquid to vapour (or vice-versa) with an acceptance probability $\boldsymbol{p_{acc} = \min[1, \exp(-\Delta H / k_B T)]}$
  - Similarly, the particles perform a random walk on wet areas of the substrate, but cannot move into dry areas.
  - The Hamiltonian from which $\boldsymbol{\Delta H}$ is obtained is as follows:

$$H = -\varepsilon_l \sum_{\langle ij \rangle} l_i l_j - \varepsilon_n \sum_{\langle ij \rangle} n_i n_j - \varepsilon_{nl} \sum_{\langle ij \rangle} n_i l_j - \mu \sum_i l_i$$

Nanoparticle Simulations



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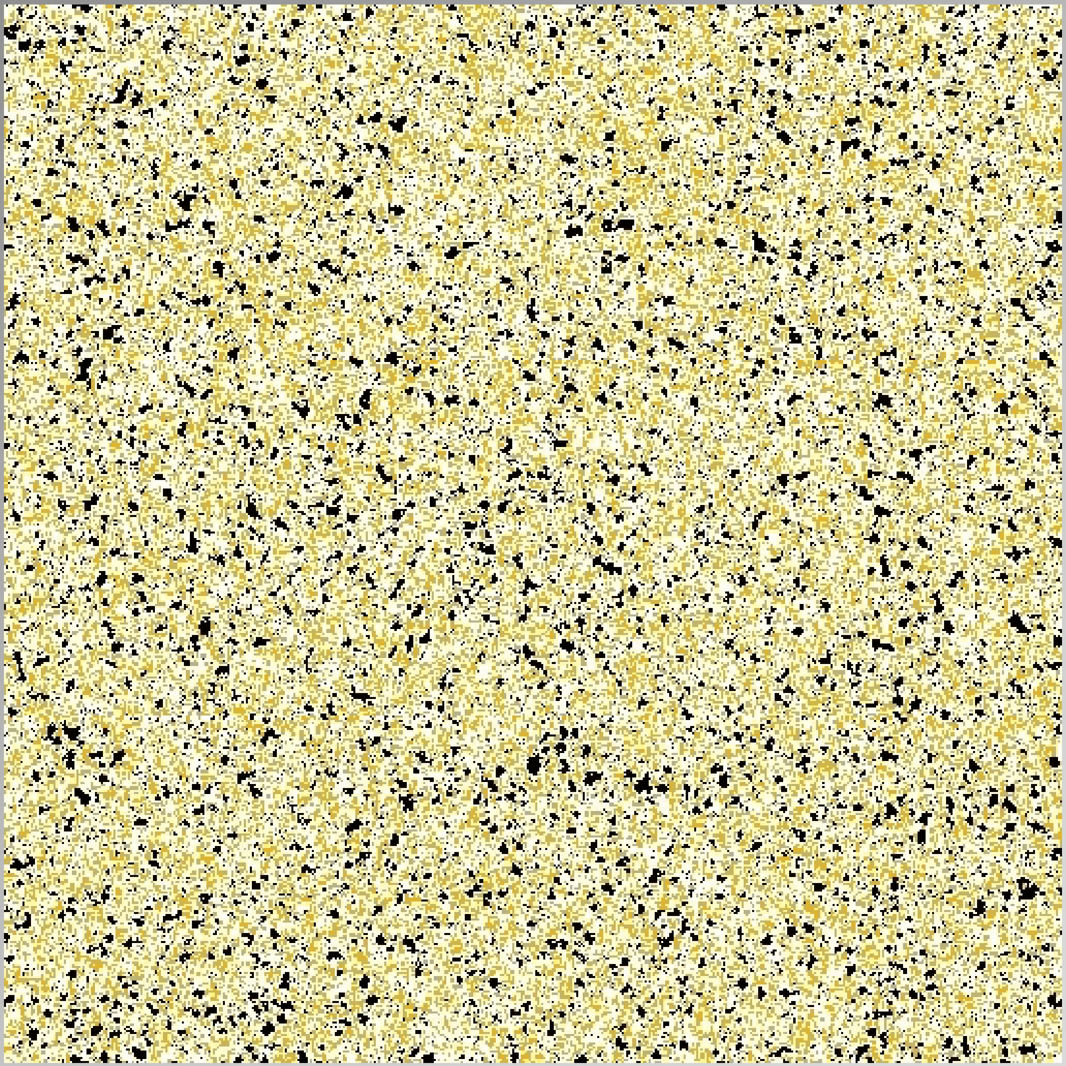
Nanoparticle Simulations



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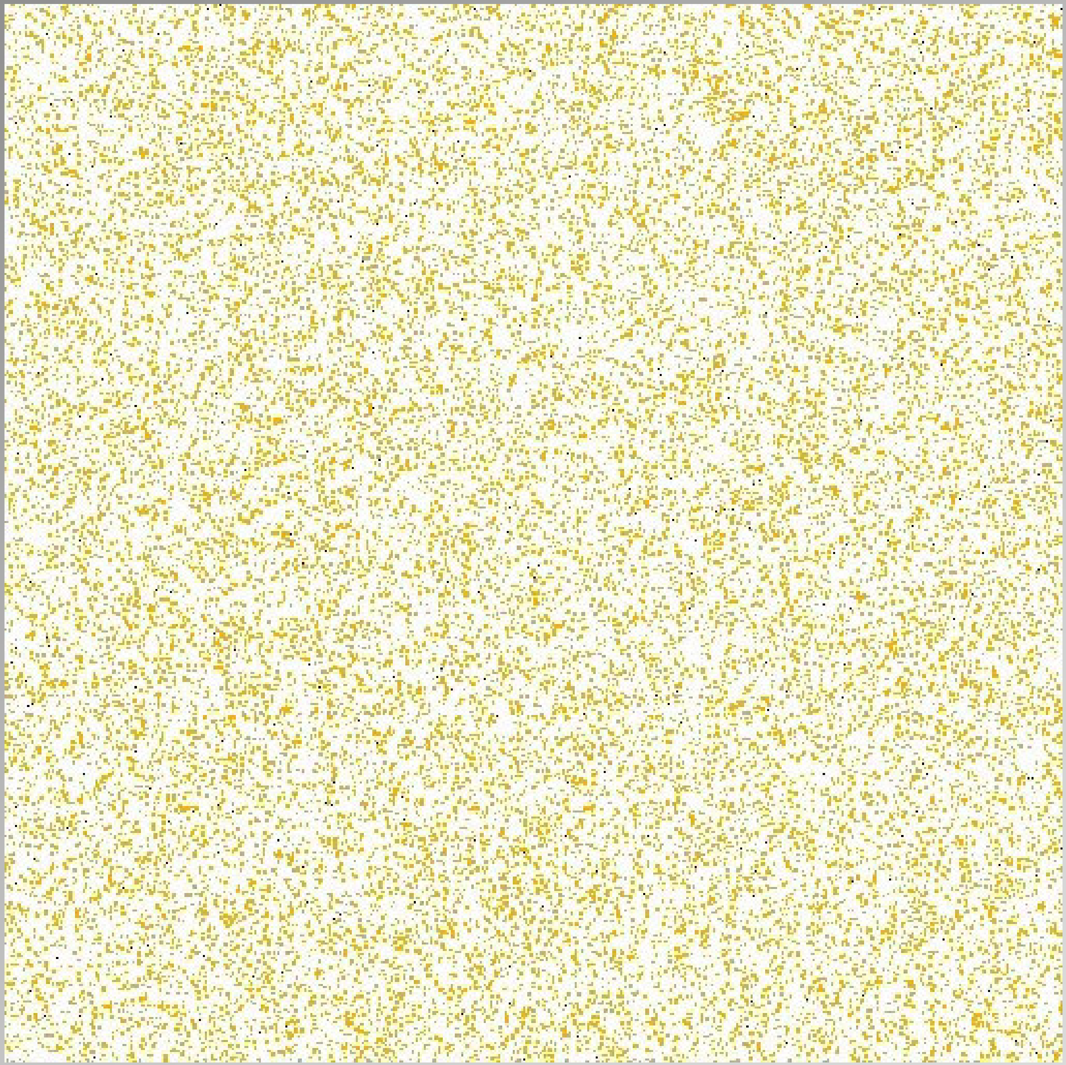
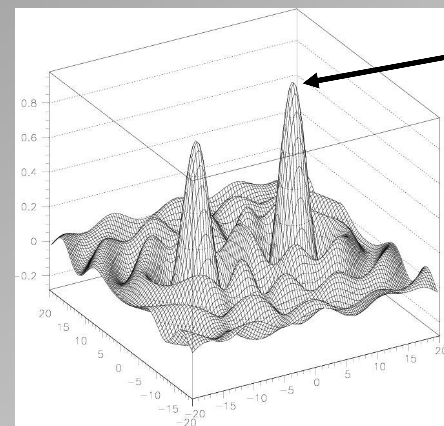


A brief overview of Genetic Algorithms

Motivation

- optimisation problems
- large search space
- inspired by Darwinian evolution



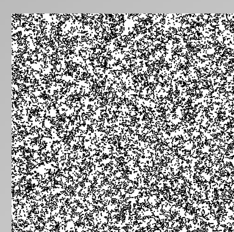
global optimum

- area covered?
- degree of order?
- similarity to target pattern?

22	0.25	1.0	4.5

genotype

simulator



phenotype

fitness function

1.05

fitness

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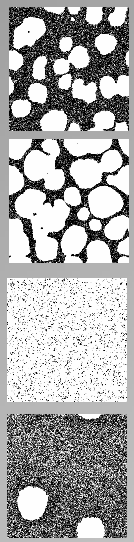
A brief overview of Genetic Algorithms

Evolution

- Recombination (mating)
  e.g. exchanging parameters
  'combine the best bits of each parent'

- Mutation
  e.g. altering the value of a parameter at random with some small probability

GENERATION 0



TIME

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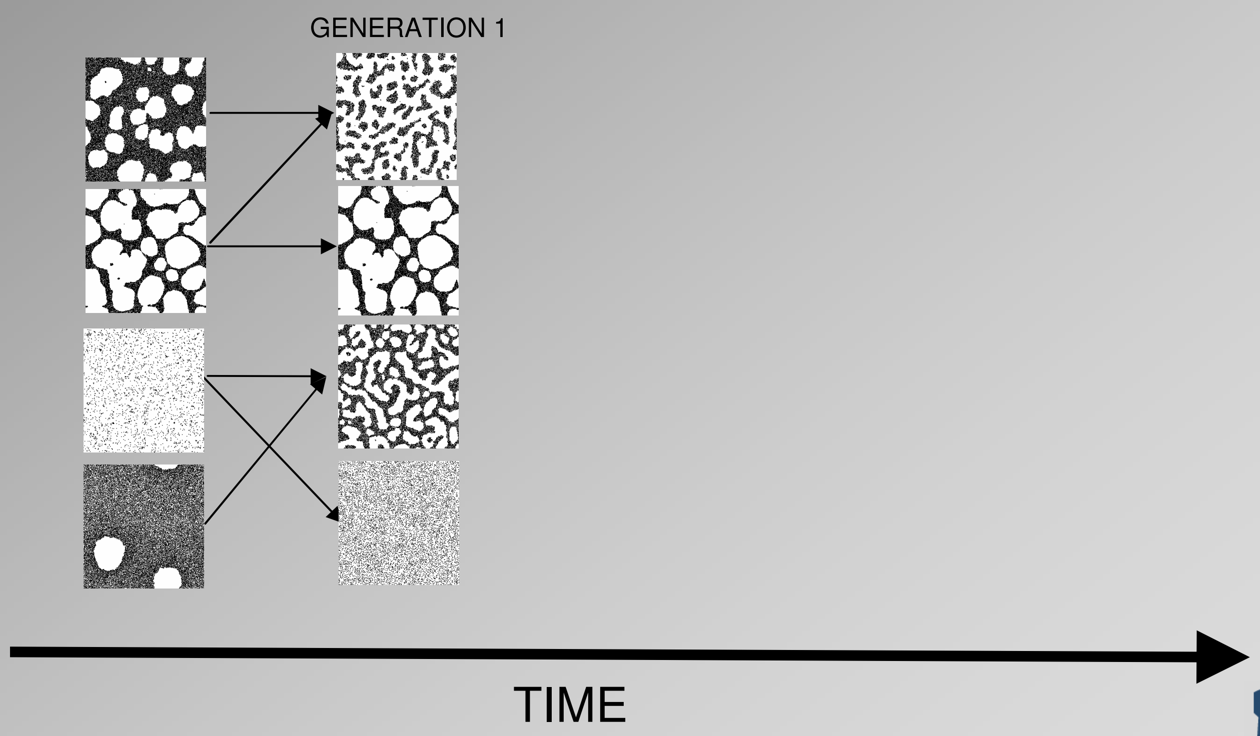

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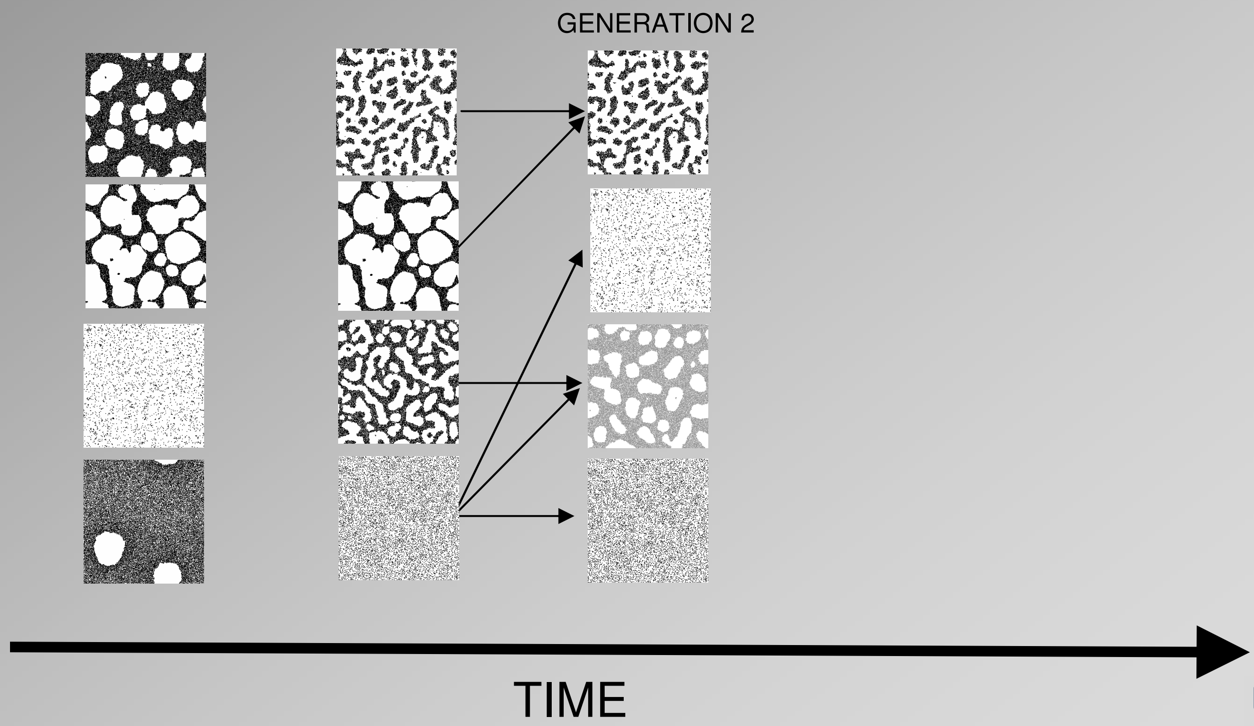

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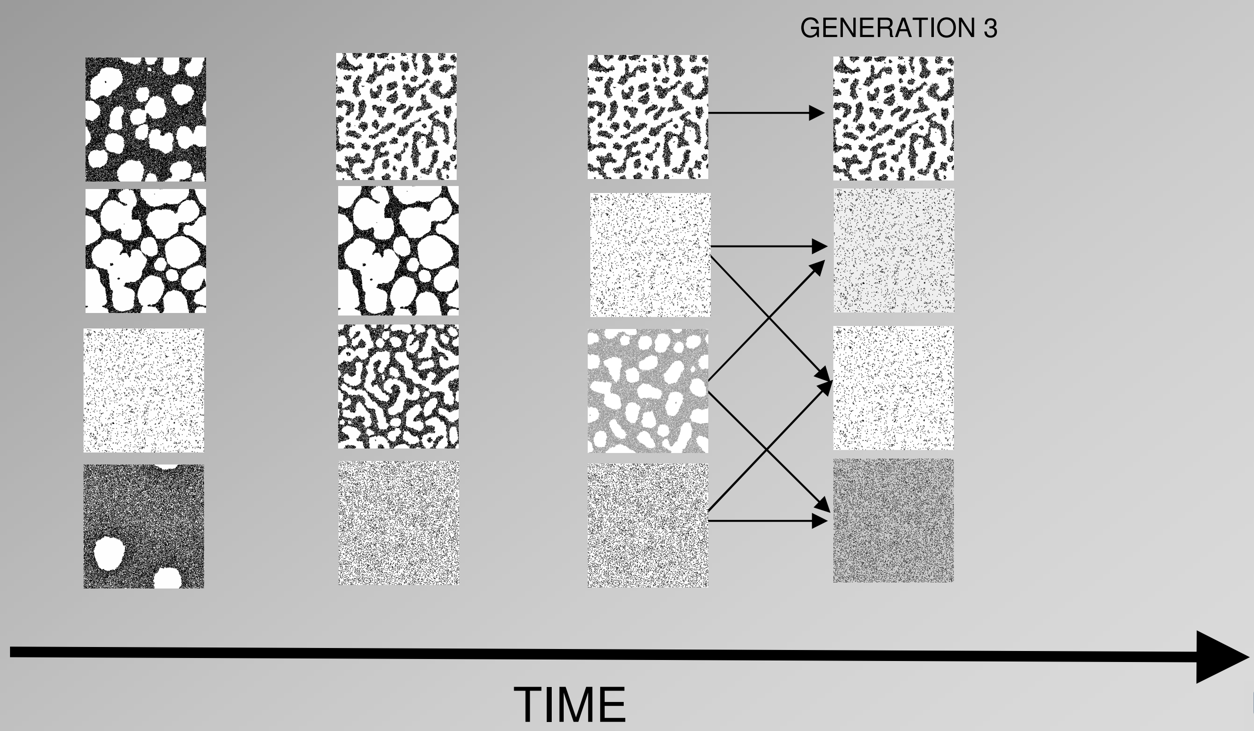

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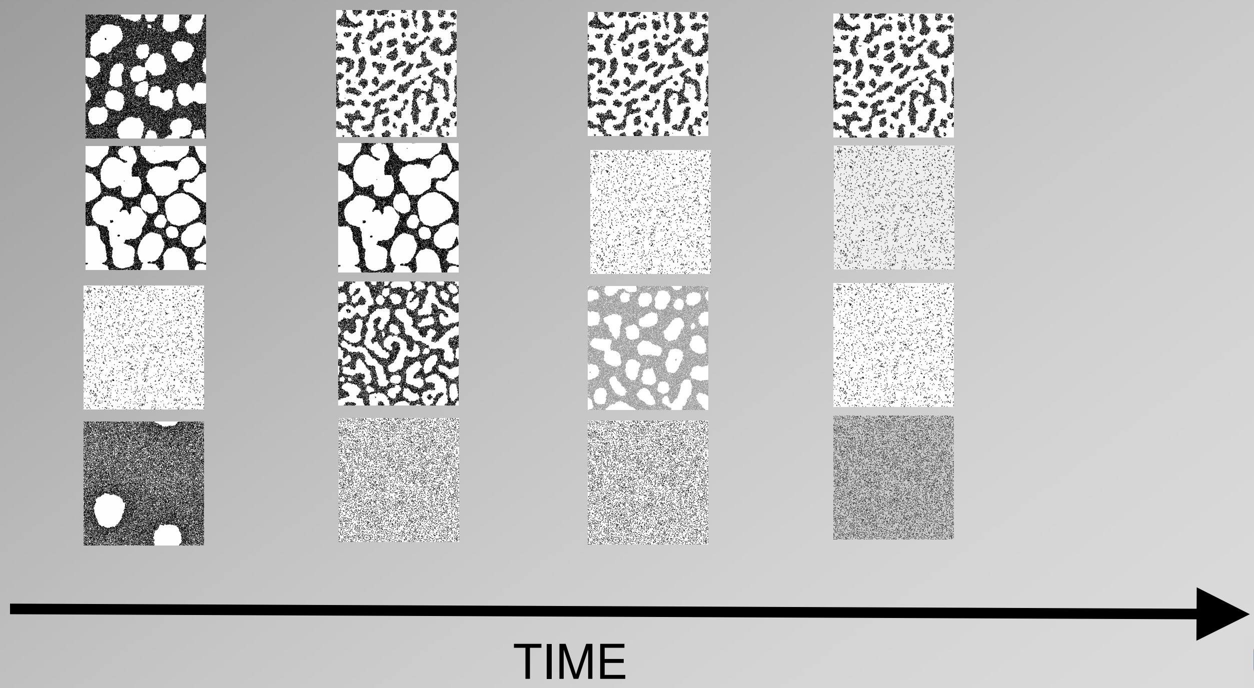

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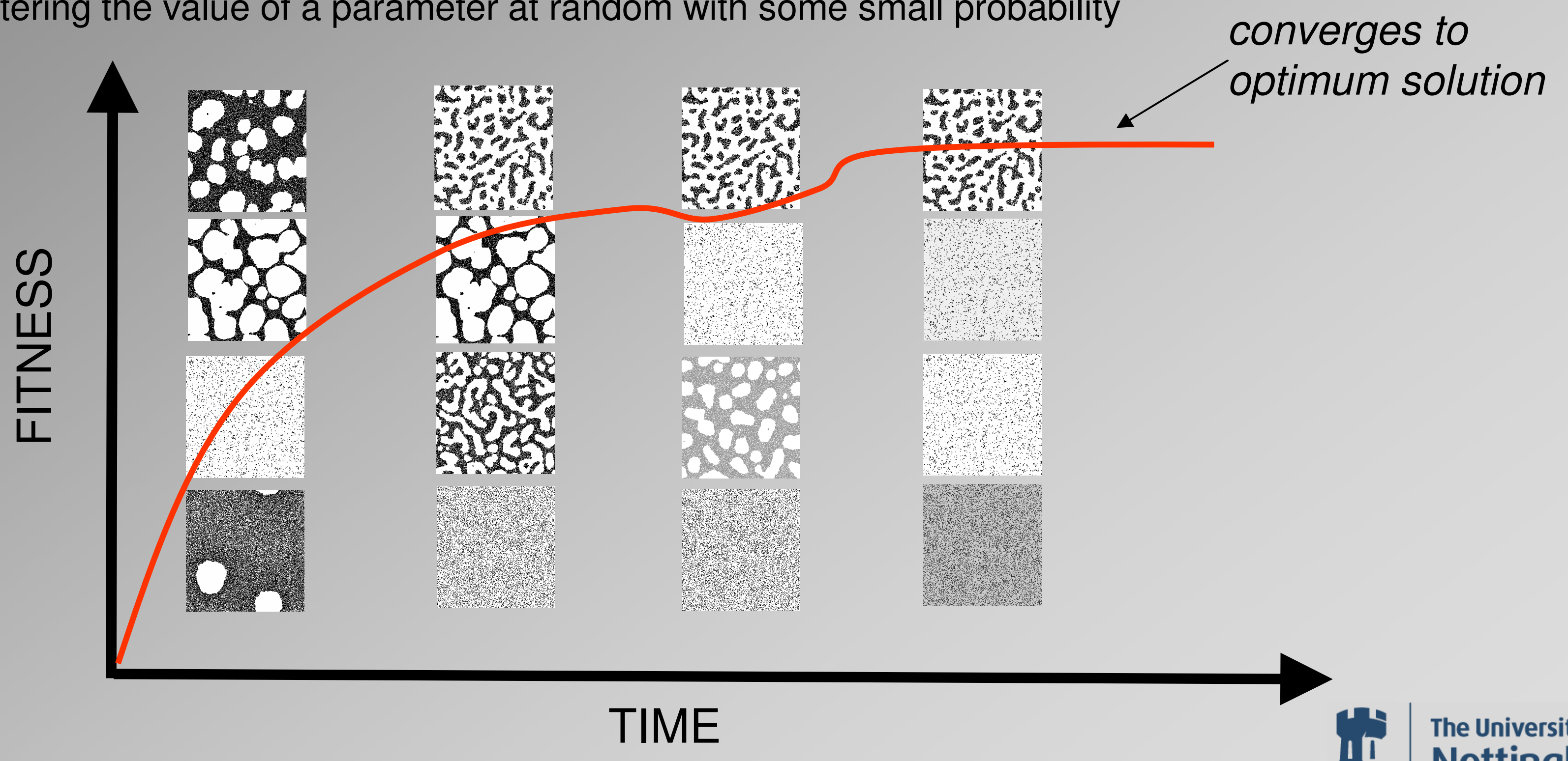


Evolving towards a target pattern

Fitness function:

"How similar is this pattern to the target pattern we are trying to recreate?"

How do we measure this?

The Universal Similarity Metric

is a measure of similarity between two given objects, o_1 and o_2, in terms of information distance:

$$d(o_1,o_2) = \frac{\max\{K(o_1 \mid o_2), K(o_2 \mid o_1)\}}{\max\{K(o_1), K(o_2)\}}$$

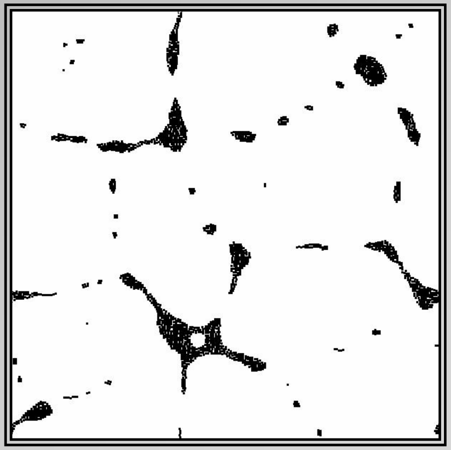
where K(o) is the Kolmogorov complexity:

K(o): The length of the shortest program for computing o by a Turing machine
$K(o_1|o_2)$: How much (more) information is needed to produce object o_1 if one already knows object o_2

Evolving towards a target pattern (simulated)

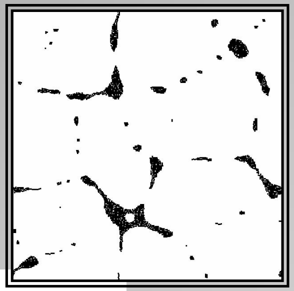
- Selected a target image from simulated data set
- Initialised GA
  - Roulette Wheel selection
  - Uniform crossover (probability 1)
  - Random reset mutation (probability 0.3)
  - Population size: 10
  - Offspring: 5
  - $\mu + \lambda$ replacement
- Ran the GA for 200 iterations
  - on a single processor server, run time ≈ 5 days
  - using Nottingham's cluster (up to 1024 nodes), run time ≈ 12 hours

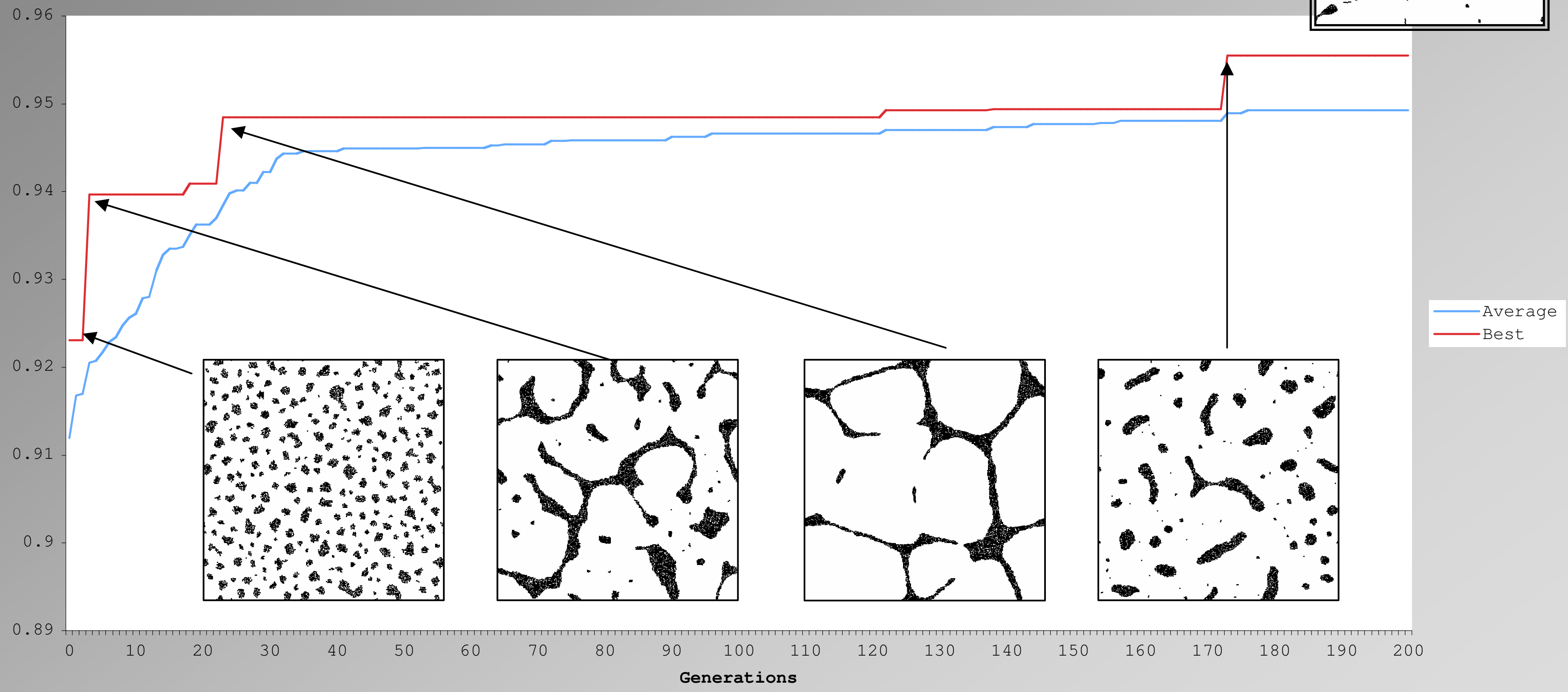
Target:



Evolving towards a target pattern (simulated)

Target:





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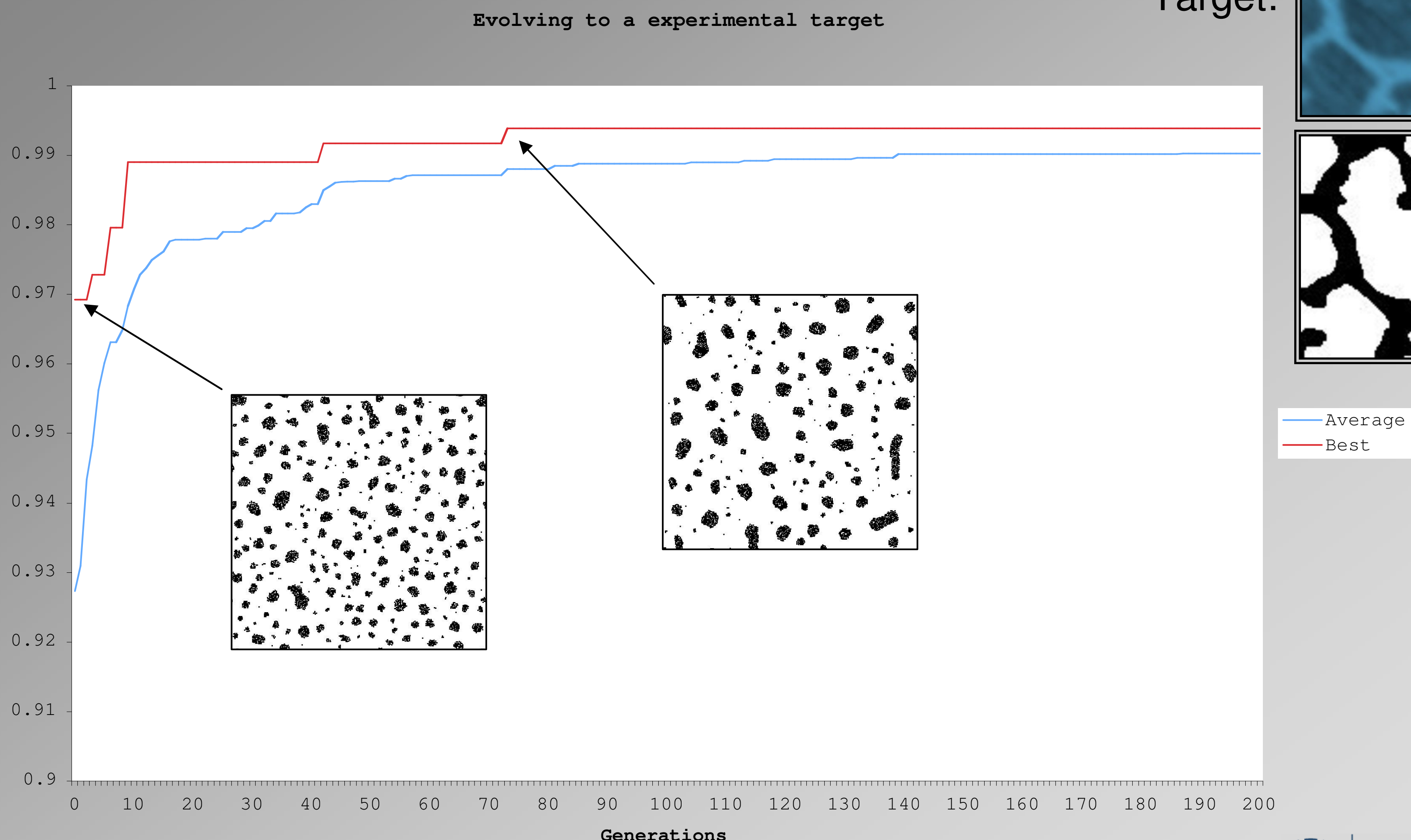
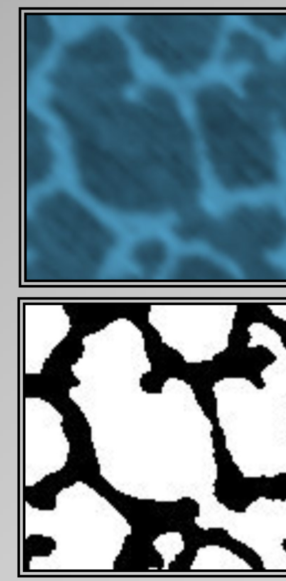
Evolving towards a target pattern (experimental)



Target:



Conclusions and further work

- we can evolve target simulated behaviour using a GA with the USM
- work continues to improve the evolution of experimental behaviour
- use of more introspective fitness functions
  e.g. Minkowski functionals

  - open ended (multiobjective) evolution

    e.g. "evolve a pattern with as many large spots as possible in as ordered a fashion as possible"
- parameter investigations
  - larger populations
- full fitness landscape analysis

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