ECM3412
Nature-Inspired Computation

Applications of Cellular Automata

Today's Plan

- Brief Recap on ALife & Cellular Automata
- Application 1: Enzyme kinetics
- Application 2: Epidemiology
- Application 3: Optimisation (Perhaps)
- Conclusions
- Examinable Reading

Artificial Life (ALife) Summary

- ALife is the simulation/synthesis of life-like forms in:
  - Wetware
  - Software
  - Hardware
- Biology is top-down
- Alife and cellular automata are bottom-up
- Alife and CA are concerned with the interaction of simple elements and emergent behaviours

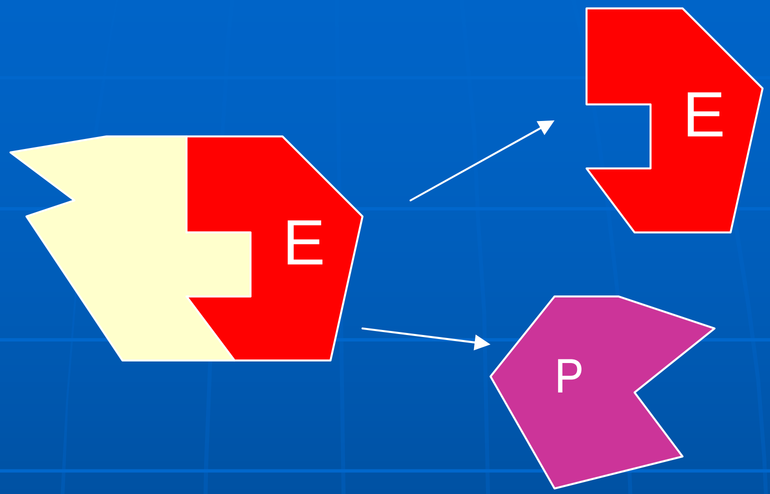
Cellular Automata

- Represented by a grid/lattice of discrete cells
- Each cell can be in a number of ‘states’
- Simulation progresses in discrete timesteps
- At each timestep the states of cells are updated by the state transition rules

Cellular Automata Applications

- CA have been applied in a large number of areas:
  - Physics
  - Fluid Dynamics
  - Plate Tectonics
  - Urban Modelling
  - Biology and Bioinformatics
- Cellular automata don’t use a fitness function, they can be difficult to apply to search and optimisation problems
- However, this is possible as we might see later
- Therefore many of the applications are efficient simulations of natural systems

Application 1: Enzyme Kinetics



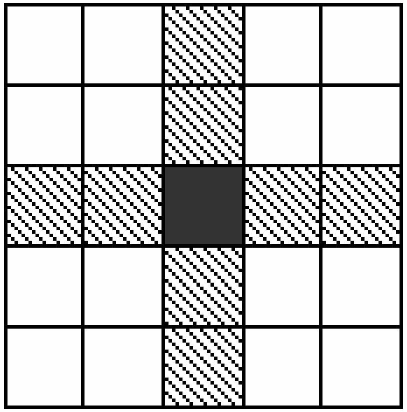
- Enzymes catalyse (speed up) chemical reactions within the body many thousands or millions of times.
- Without enzymes, life could not exist
- For instance, without enzymes it would take weeks to digest food, by which time we'd be dead
- The enzyme works (for the purposes of this application) by locking onto it's target (known as the substrate), catalysing the reaction and releasing the product(s)

Cellular Automata Models for Enzyme Kinetics (Kier et al, 1996)

- Better understanding of the reaction between enzyme and substrate could help us to better understand the large number of enzyme-involved processes in the cell.
- Enzyme reactions are dynamic, and even with frequent experiments, the dynamic process cannot fully be seen.
- Modelling may provide the solution.

Cellular Automata Models for Enzyme Kinetics (Kier et al, 1996)

- The cellular automaton consists of:
  - **Grid -** 110*110 grid of cells
  - **States -** Each cell can have one of four states:
    - Enzyme (E)
    - Substrate (S)
    - Product (P)
    - Water (W)
  - **Neighbourhood -** Each cell has an extended von Neumann neighbourhood.
  - **Rules -** Each cell has associated with it, the probability of its movement and interaction with other molecules in the CA.



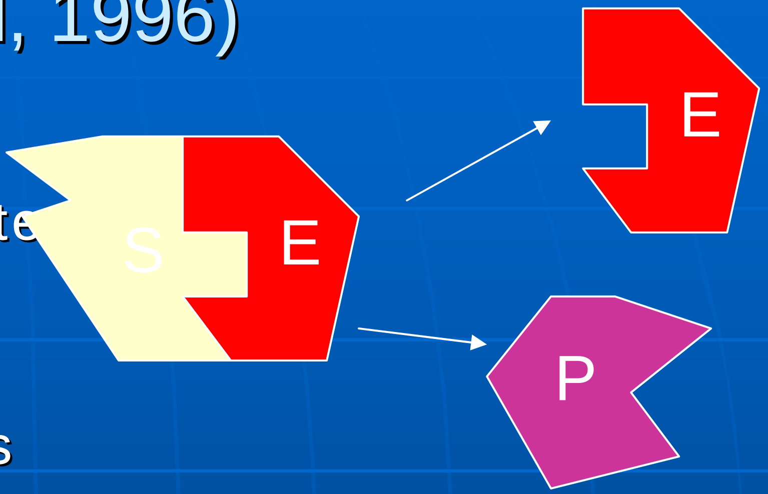
Extended von Neumann Neighbourhood

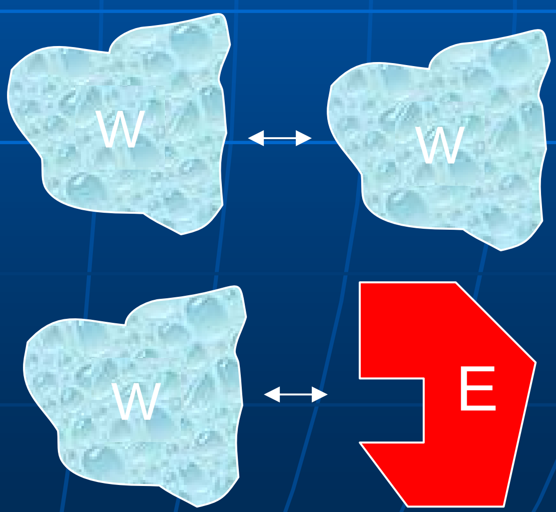
Cellular Automata Models for Enzyme Kinetics (Kier et al, 1996)

- Initialisation – the grid is filled with 69% water and 31% unused space. When other ingredients are added, they replace the water, so the cavity ratio is maintained
- Each of E,S,P and W have:
  - A probability of joining (moving towards) other molecules in the neighbourhood.
  - A probability of breaking (moving away) from the other molecules
  - The movement probability. A probability of 0 indicates a stationary enzyme.
- Each enzyme can join with one molecule of either S,P or W, but not another E.

Cellular Automata Models for Enzyme Kinetics (Kier et al, 1996)

- A further parameter gives a probability for an enzyme-substrate complex turning into an enzyme-product complex.
- Once the enzyme has reacted, this is an irreversible process.
- The water-breaking parameter can be seen as a substitute for temperature in the system.
- The breaking parameter between other molecules and water determines their hydrophobicity





Cellular Automata Models for Enzyme Kinetics (Kier et al, 1996)

- These CA parameters were used:
  - Water "Temperature" set to simulate human body temperature
  - Run several hundred times to discover the impact of parameter settings
- These parameters were found to replicate the Michaelis-Menten kinetics of enzyme reactions for enzyme reactions.
- The cellular automaton model enables:
  - The user to monitor the concentration of each of the molecules at any timestep
  - The user to change the concentration of any of the molecules and see the effect on the system

Conclusions

- Cellular automata can provide a model of biochemical processes where the parameters can be changed
- Not easy to see how this might be done without CA and would require complex equations.
- Interesting philosophical point – artificial life simulating real life

Epidemiology Applications

- Spread of disease (epidemiology) can be effectively modelled by cellular automata
- Cells represent points in space and could be occupied or not-occupied by potentially disease carrying agents (e.g. humans or birds)
- The points in space can be at a different scale:
  - Confined space e.g. waiting room/train platform
  - City
  - County
  - Country
  - Worldwide

Epidemiology with CAs

- There are standard methods for simulating the spread of disease.
- Each cell can take a variety of states:
  - Occupied (by N individuals)/Not Occupied
  - If occupied, then the individual(s) can be:
    - S – Susceptible
    - I – Infected
    - R – Recovery
- Type and size of neighbourhood will be dependent on the scale of the simulation and the infectiousness of the disease

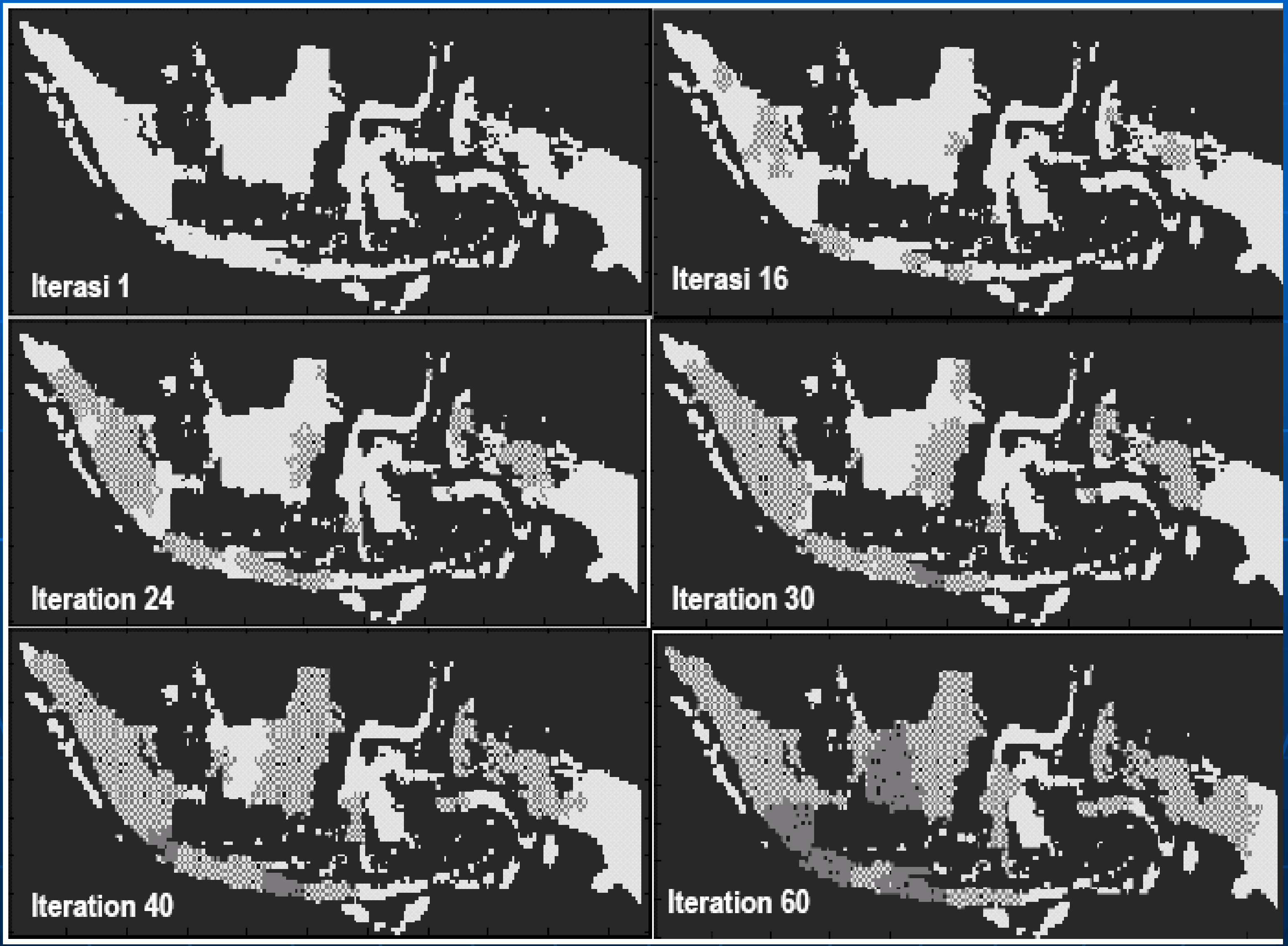
Epidemiology Parameters

- The model parameters can be set up to simulate agent (avian or human) movements between cells by modifying the speed of state change

- Other parameters can be changed by subtly changing the state transition rules to reflect the disease:
  - Infectiousness (how easily susceptible individuals become infected)
  - Infectious period
  - Possible re-infection after recovery?
  - Morbidity rate

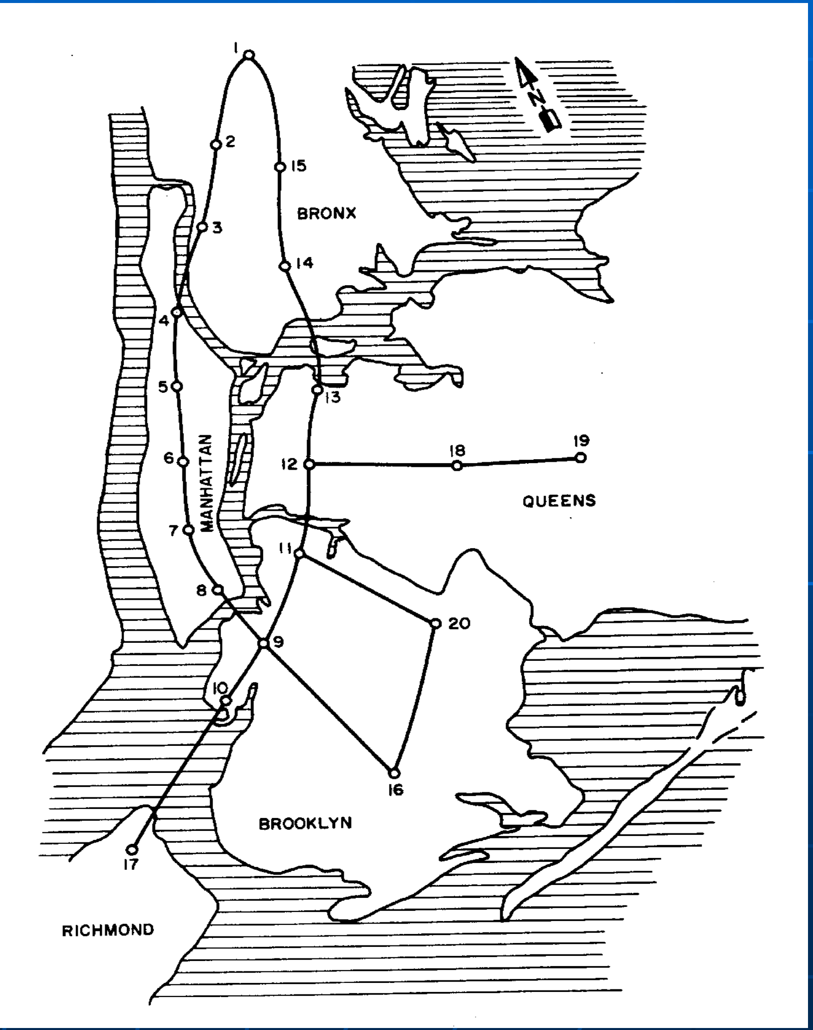
- How could you modify the state transition rules to reflect these properties?

Graphical Plot of CA for Epidemiology of Avian Influenza in Indonesia (Situngkir, 2004)



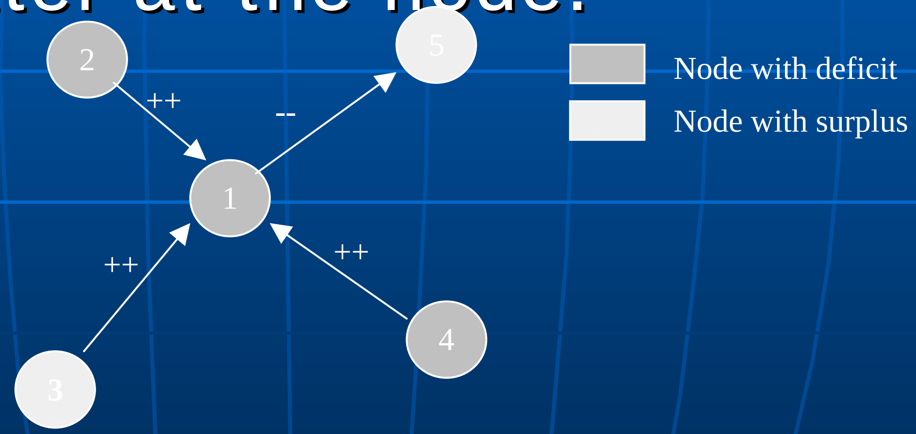
Application 3: Water Distribution Network Optimisation (Savic & Walters, 1997)

- Water distribution networks consist of a set of pipes, nodes, tanks reservoirs, pumps and other elements.
- They must distribute water from a source to the nodes, where people use it.
- The size of the pipes used in the network have an impact on the fitness of the network, broadly speaking:
  - Larger pipes = more water but greater cost to make and install
- EAs have been used to find a near-optimal set of pipes sizes for a network



CAs for WDN Optimisation

- Each cell is represented by a pipe and a node.
- The pipe size is incremented if there is not enough water at the node
- The pipe size is decremented if there is too much water at the node.



- Applied to all the nodes in the network at once.

CAs for WDN Optimisation

- Therefore, the network attempts to 'self organise' to meet the requirements dictated at the nodes (consumers consuming water).

- Can get quite close to EA solutions whilst evaluating a fraction of the solutions:
  - CA – 5-20 evaluations
  - EA – 25k+ evaluations

Overall Conclusions

- Cells can be used to represent almost anything but are mostly spatially located:
  - Microscopic locations in a cell
  - Locations in a country
  - Abstract locations in a network
- The way in which the automata works is determined by the selection of
  - Neighbourhood
  - States
  - State Transition Rules