Rule-based modelling with the XL/GroIMP software

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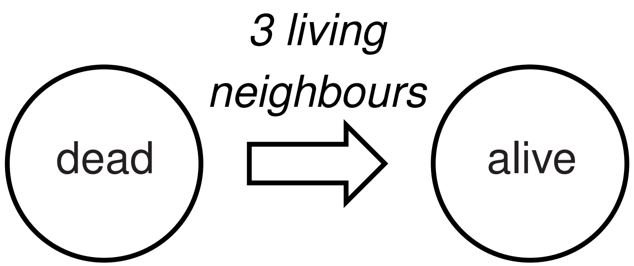
Motivation

- Models of biology or ALife are often specified in a rule-based manner.
- This *natural choice* of specification is lost in a conventional implementation:

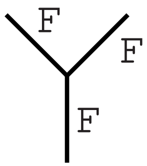



```
for (x = 0; x < n; x++) {
    for (y = 0; y < n; y++) {
        sum = 0;
        for (dx = -1; dx <= 1; dx++) {
            for (dy = -1; dy <= 1; dy++) {
                if (((dx != 0) || (dy != 0))
                    && state[(x + dx) % n][(y + dy) % n])
                    sum++;
            }
        }
        if (!state[x][y] && (sum == 3))
            newState[x][y] = 1;
    }
}
tmp = newState;
newState = state;
state = tmp;
```

- A rule-based language reflects the nature of such models in a much more concise way.

Rule-based modelling: L-systems

L-systems, established in 1968, provide a rule-based formalism. They are used in biological modelling.

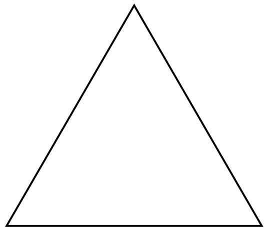
- Data structure: Linear *string* of symbols, e.g.,
  `F [ + F ] [ − F ]`
- Turtle graphics interpretation leads to
  3D-structures: 

- String replacement rules implement dynamics:
  `A ⟶ F [ + A ] [ − A ]`
  Thery are applied in parallel.

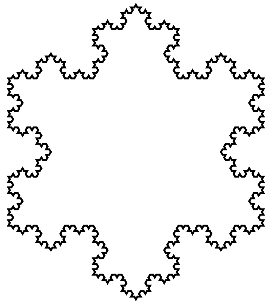
Von Koch curve as an L-system

The von Koch (snowflake) curve arises out of the following L-system

$$\alpha \longrightarrow \mathtt{F} + + \mathtt{F} + + \mathtt{F}$$
$$\mathtt{F} \longrightarrow \mathtt{F} - \mathtt{F} + + \mathtt{F} - \mathtt{F}$$



F++F++F



The software *GroIMP* displays these derivation steps.

- The input is the L-system itself: Thus, specification and implementation are congruent.
- User interactions are possible.

L-system examples of biology

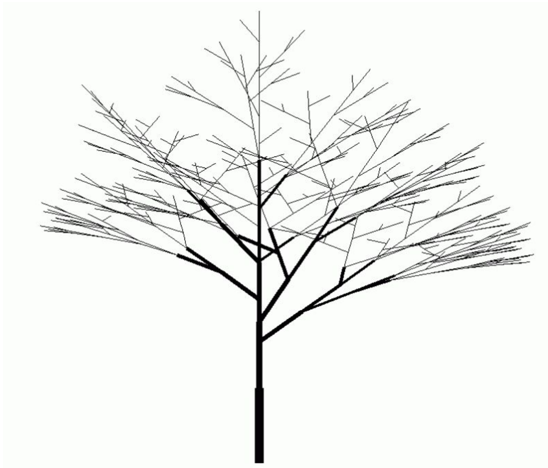
Main field of application of L-systems: Biological modelling, especially of *plant morphology*.

- Plant growth can suitably be described as a *rule-based* process.
- Realistic images can be produced.

```
* # f(-30) RL(90) f(800) RL(-90) a(10,1)
a(l,w) # D(w) F(l) [ RL(a0) b(l*r2, w*wr) ] RH(d) a(l*r1, w*wr)
b(l,w) # D(w) F(l) [ RU(a2) $ c(l*r2, w*wr) ] RH(d) c(l*r1, w*wr)
c(l,w) # D(w) F(l) [ RU(-a2) $ b(l*r2, w*wr) ] RH(d) b(l*r1, w*wr)
```

A parametric tree

$\Rightarrow$



Some L-system-generated images

Disadvantages of L-systems

L-systems have a number of disadvantages:

- Linear (1D string) data structure.
- Objects are simple symbols.
- Expressiveness of rules is limited.

These drawbacks become essential when modelling complex structures and interactions:

- Complex structures do not fit well into the linear world of strings.
- Complex interactions on string-encoded structures are not reasonably realizable.

Current solutions

Current solutions “outsource” the complexity:

- Prusinkiewicz introduced *open* L-systems which can be coupled to external programmes (software cpfg, L-Studio).
- Kurth introduced *sensitive* L-systems which provide a number of predefined environment functions (software GROGRA).

A better solution would be the enhancement of expressiveness of the rule-based language! This can be achieved by the transition from *strings* to *graphs*.

Graphs and graph grammars

Graphs are sets of nodes and connecting edges.

- This includes L-system-like strings as a subcase.
- General structures can be encoded immediately.
- Graph query languages extract information.

Graph grammars are rewriting systems that operate on graphs.

- Again, L-systems are a subcase.
- Complex model dynamics can be implemented in a concise way using graph transformations.

Relational Growth Grammars

Relational Growth Grammars (RGG) are graph grammars, primarily tailored to the needs of modelling plant growth.

- Edge-labelled directed graphs build the data structure, nodes are objects of the underlying programming language.
- A conventional programming language is included.
- Graph queries can be formulated.
- Relations can be defined and used in queries.
- This general framework is also suitable for ALife.

XL: An implementation of RGG

XL is a Java-based implementation of RGG for the use in practice.

- Most constructs of Java have been integrated (classes, methods, variables, loops, ...).
- Graph transformation rules and queries can easily be formulated.
- Certain Java classes serve as turtle commands.
- All existing Java runtime libraries can be used.
- XL is integrated in the software *GroIMP*.

Von Koch curve as an RGG-system

The snowflake L-system as an RGG-system:

```
class Koch extends RGGSystem {
    void run() [
        Axiom ==> F(1) RU(120) F(1) RU(120) F(1);
        F(x) ==> F(x/3) RU(-60) F(x/3) RU(120) F(x/3) RU(-60) F(x/3);
    ]
}
```

Specification and implementation are nearly congruent:

- An enclosing Java-like code is needed.
- Apart from that, the L-system is implemented in a 1:1 fashion.

Game Of Life: Specification

Conway's Game Of Life is specified as follows:

- The world is a 2D two-state (*dead* or *alive*) cellular automaton with Moore-neighbourhood.
- A living cell dies if it has less than two, or more than three living neighbours.
- A dead cell becomes alive if it has exactly three living neighbours.

The specification can be written down in three lines.

Game Of Life: Implementation

Geometrical definition of neighbourhood:

```
iterating Cell neighbours(Cell c1) {
    yield (* c1 -+- #c2:Cell, (c1.distanceLinf (c2) < 1.1) *);
}
```

Transition rules:

```
void transition() [
    x:Cell(1), (!(sum(neighbours(x).state) in {2..3})) ==>> x(0);
    x:Cell(0), (sum(neighbours(x).state) == 3) ==>> x(1);
]
```

- The original specification is reflected concisely in the implementation.

Making use of relations

Definition of neighbourhood as a relation:

```
boolean neighbour(Cell c1, Cell c2) {
    return (c1 != c2) && (c1.distanceLinf(c2) < 1.1);
}
```

Modified transition rules:

```
void transition() [
    x:Cell(1), (!(sum((* x -neighbour-> #Cell *).state) in {2..3}))
        ==>> x(0);
    x:Cell(0), (sum((* x -neighbour-> #Cell *).state) == 3) ==>> x(1);
]
```

- Such a *relational view* may help to increase the readability of implementation code.

The modelling platform GroIMP

GroIMP is designed as an integrated modelling platform:

- XL grammars can be interpreted.
- Classes useful in modelling are provided: Turtle commands, further geometrical classes, cells, ...
- The outcome of a model is visualised.
- User interaction during the simulation is possible, even over a network.

GroIMP is still under development.

A simple ant model

A simplistic ant simulation is implemented easily:

- Ants live in a rectangular grid world.
- Ants release pheromone while moving.
- Released pheromone decays by and by.
- Ants remember the last twenty cells visited.
- The movement is influenced by the reachable pheromone values, a direction-preserving tendency, the memory and a random effect.
- There are food sources which stimulate the pheromone deposition of ants.

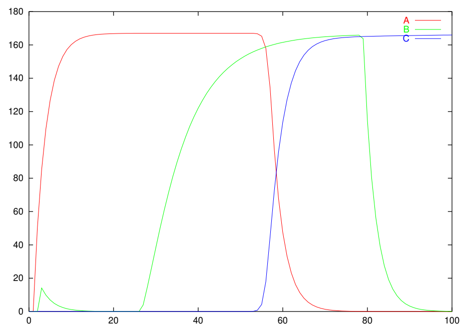
Ant model implementation

```
class Ant extends Cylinder {
    float dx, dy; // current moving direction
}

class AntSimulation extends RGGSystem {
    const int memory = MIN_USER_EDGE; // a user-defined edge

    boolean placeAntAt(int i, int j) { where to place ants initially... }

    float evaluate(float pheromone, float dirdelta2) { evaluation of a possible move...
        // pheromone: Pheromone content of the reached cell,
        // dirdelta2: squared difference of the direction vectors }

    void run() [
        // move ant a to next cell, keep current cell c in memory with counter value 20
        c:Cell a:Ant ==>> n:nextCell(c, a) a -memory-> 20 c
                   { a.dx := n.x - c.x; a.dy := n.y - c.y; // update moving direction
                     float p = (a.length + c.state) * C_ANT; // amount of pheromone laid down
                     a.length :+= c.state - p; // update ant excitation status
                     c.length :+= p; // lay down pheromone };

        // decrease the memory counter; if it has reached zero, the memory node is removed
        m:int ==>> if (m > 0) m(m-1);

        c:Cell ::> c.length :-= c.length * C_CELL; // decay of cell pheromone
    ]

    Cell nextCell(Cell c1, Ant a) {
        float dx, dy;
        // find the neighbouring cell c2 not in memory with maximum evaluate-value:
        Cell next = select((* c1 -+- #c2:Cell,
                              (c1.distanceLinf (c2) < 1.1),
                              (!exist((* a -memory-> int c2 *))) *),
                           (dx = (c2.x - c1.x) - a.dx, dy = (c2.y - c1.y) - a.dy,
                            evaluate(c2.length, dx * dx + dy * dy)) -> max);
        return (next != null) ? next
                              : c1; // all neighbours are in memory, ant doesn't move
    }

    void init() [
        // create a 25 * 25 grid of cells, place the ants
        Axiom ==>> ^ for(i = 0 .. 24) for(j = 0 .. 24) ([Cell(i, j) if(placeAntAt(i, j)) Ant]);
    ]
}
```

Back to biology: ABC model

The ABC model predicts flower morphogenesis on the basis of a genetic regulatory network.

- Three genes, A, B and C, are used.
- Their transcription factors determine the type of flower organ to be formed.
- Factor concentrations change in time.



$\Rightarrow$

$$\boxed{\begin{array}{lcl} [b] > 80, [c] > [a] & \longrightarrow & \text{stamen} \\ [b] > 80, [c] \leq [a] & \longrightarrow & \text{petal} \\ & \dots & \end{array}}$$

$\Rightarrow$

ABC model implementation

The XL implementation of the ABC model benefits from the new features of RGGs:

- The regulatory network is represented as a graph.

```
agene:Gene(0.1) -encodes-> a:Factor(0, 0.3),
a Activate(1e-9, 50) agene, ...
```

- Its dynamics is implemented using update rules.

```
f:Factor(c, d) ::> f.concentration :-= c * d;
f:Factor <-encodes- g:Gene(ct) ::> f.concentration :+= Math.max(0,
    sum(((* Factor(c2,) Activate(s, m) g *), m*c2 / (s+c2))) + ct);
```

- Morphogenesis is modelled in an L-system style.

```
m:Meristem (* -factors-> Factor(a,) Factor(b,) Factor(c,) *) ==>
  { int t = (b > 80) ? ((c > a) ? STAMEN : PETAL) : ...; }
  if (t == SHOOT) (F(0.5, 0.6)) else if (t == PEDICEL) (...) ... m;
```

A barley model

- Morphogenesis is modelled in an L-System style.
- Diploid genome controls ear morphogenesis.
- A metabolic network in each internode organ controls internode elongation.

Conclusion and outlook

In principle, RGGs provide a concise way of implementing biological or ALife models:

- Necessity of technical code has been reduced.
- The structural view of L-systems is preserved.
- Further models have to be checked.

For practice, runtime efficiency has to be acceptable.

- Graph grammars introduce a runtime overhead.
- Matching algorithm has to be improved, e.g., search order optimization or caching of matches.
- Java byte-code generation is desirable.