Graph-oriented modelling of multiscaled dynamical systems with a dynamical structure:

Challenges to the "Relational Growth Grammar" approach

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1. **Multiscaled structures**

   (≅ different views on the same structure)

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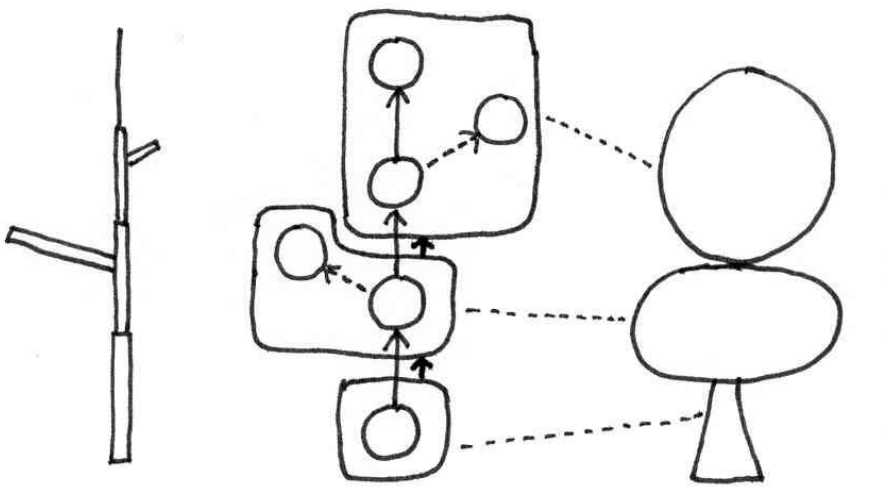

morphological structure

crown layers

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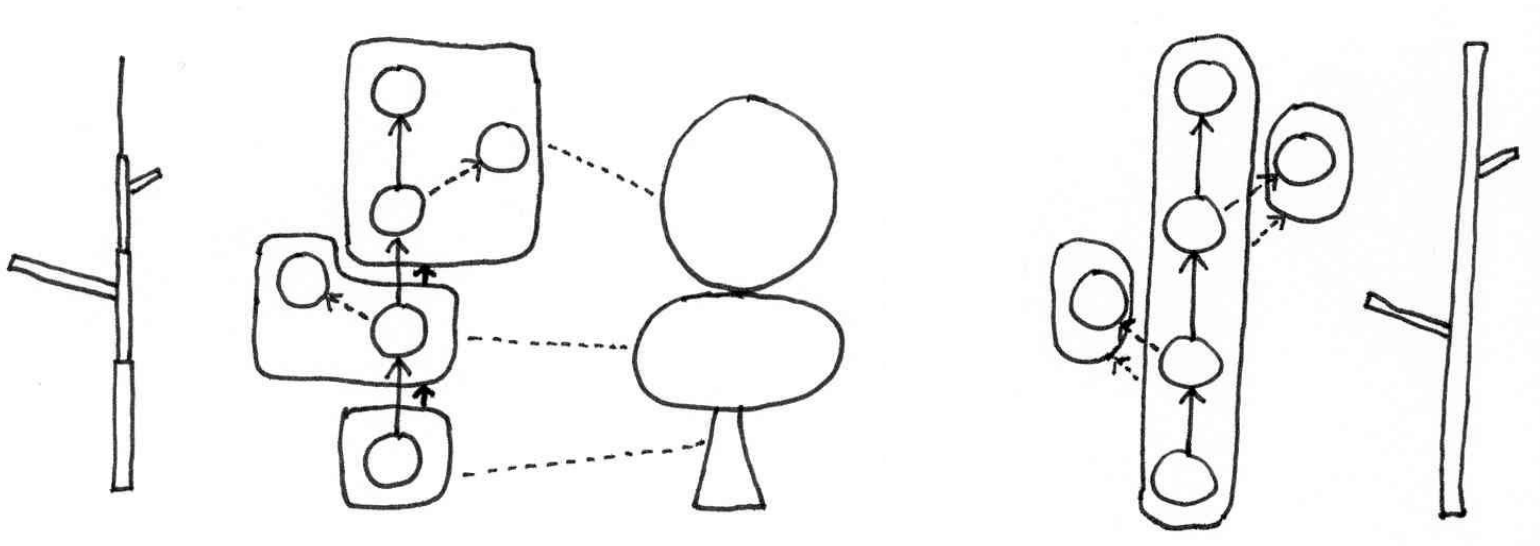

morphological structure

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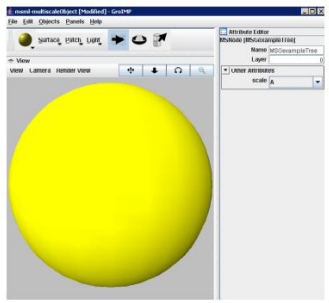
axis structure

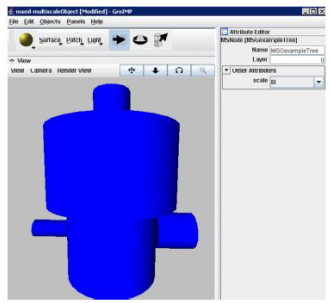
"Multiscaled Tree Graphs" (MTG):

Theoretical basis given by Godin & Caraglio 1998.

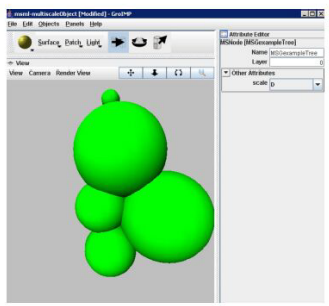
first attempt to integrate this in GroIMP: Diploma thesis by Sören Schneider (2006)



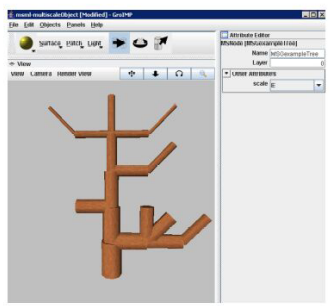
(a) Skale A



(b) Skale B



(c) Skale D



(d) Skale E

- including new XML-based data format (MSML)

- but not yet satisfactorily finished and not yet well supported

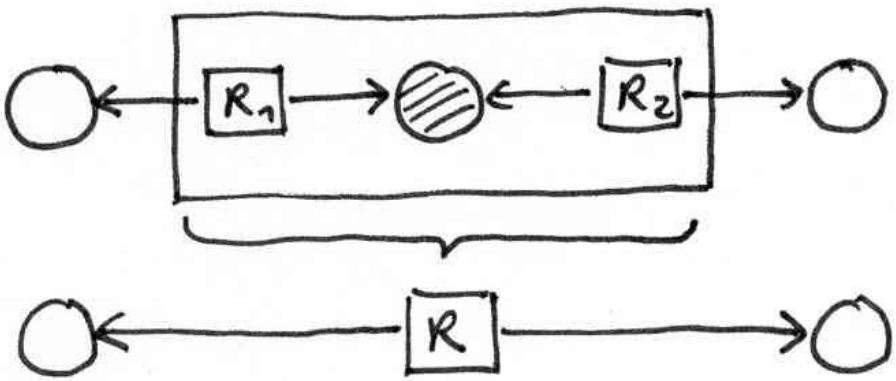
To be done:

- Extension of existing representation to all sorts of modules,
- particularly: 3D representation of structures from MTG files
- operations on aggregate modules *(e.g., complete deletion in case of a collision)*
- local adaptation of resolution (zoom-in, zoom-out)

- solution of the runtime problems of the current MTG filter of GroIMP (XSLT is too slow)

multiscaled structures are common in biochemical networks:

different resolutions of reaction chains



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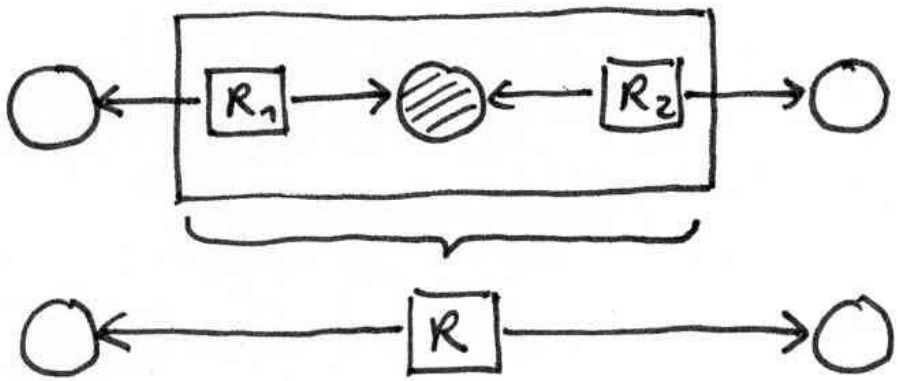


Remark:

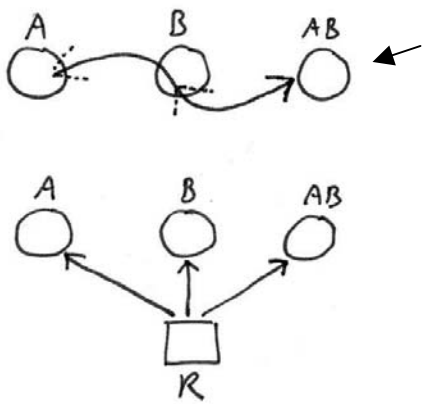
Representation of metabolic networks favorably with Petri nets.

Nodes: Substrate nodes and reaction nodes

Example:

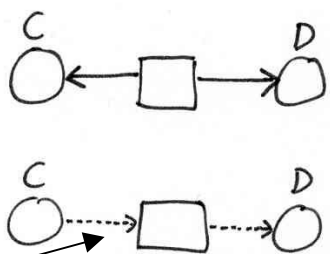
Reaction

A + B ⇆ AB



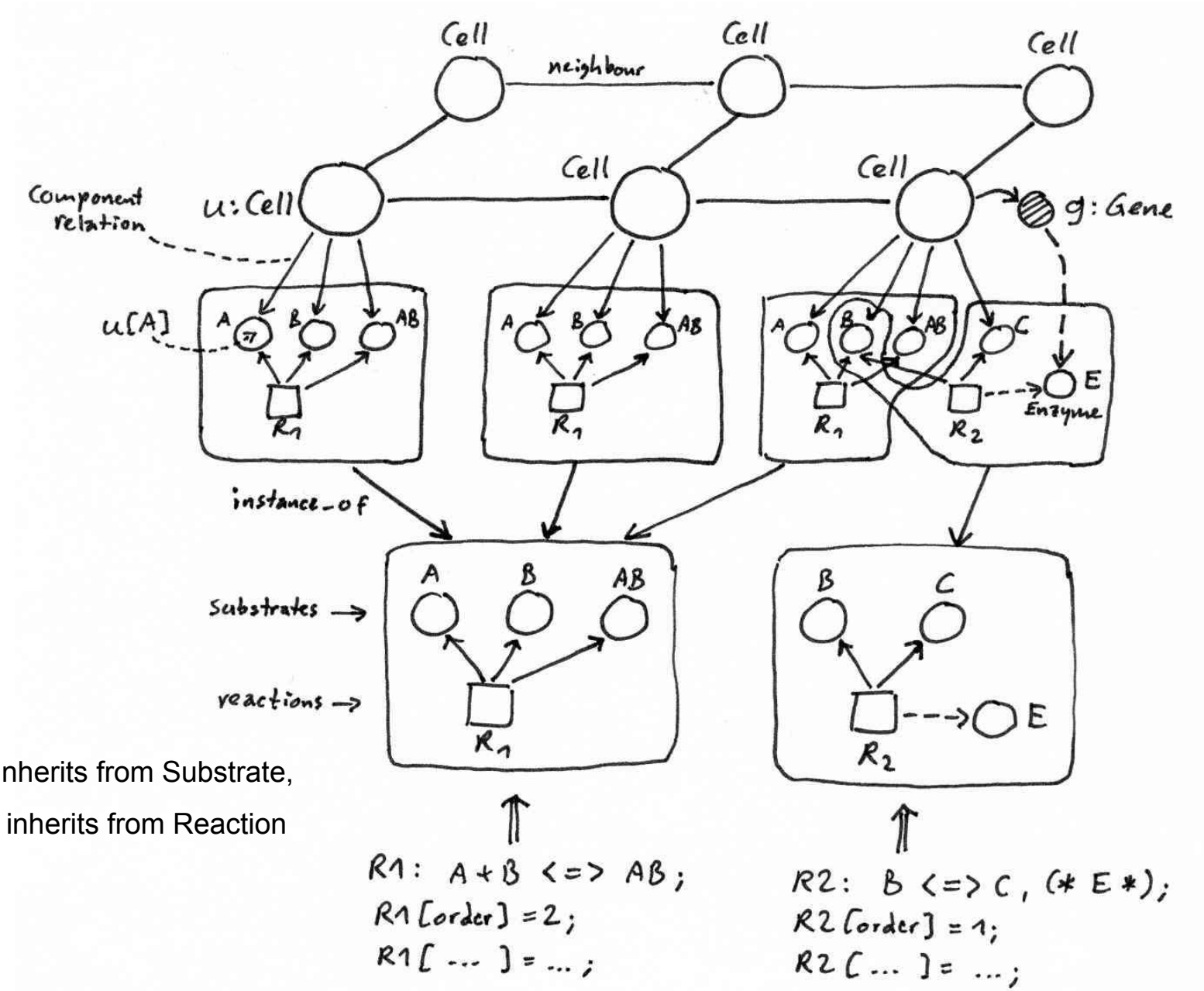
hyperedge:
not really well suited

C → D:



flow of matter

2. Instantiations of metabolic networks



3. Easy specification of sensitivity

e.g., collision detection:

A ==> F [RU(45) F B] F A;

this rule shall be applied only when none of the 3 Fs hits an existing object in space

suggestion:

A ==> b: (F [RU(45) F B] F A); /* trial */

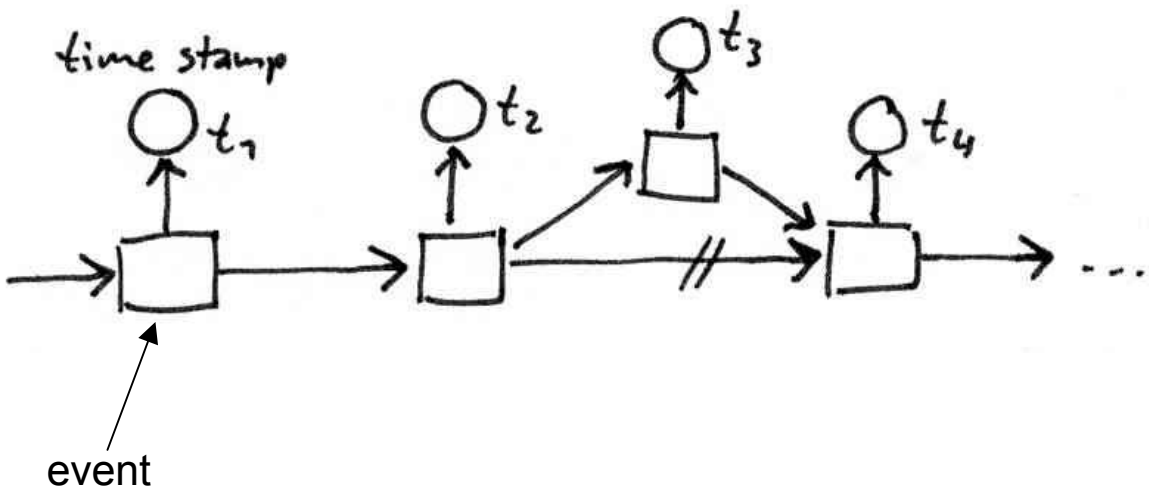
b:Compound (b.collision) ==> ; /* deletion */

4. Event queues

- or, more generally:
  a more flexible time management

RGGs use discrete time steps of fixed length

to be preferred for realistic models: continuous time (faked), event handling



- timed L-systems (Prusinkiewicz & Lindenmayer)
- differential L-systems (D0L-systems) (Prusinkiewicz et al.)
- scheduling mechanisms in SIMULA and other languages

to be developed:

a concept for general representation of dynamics in XL

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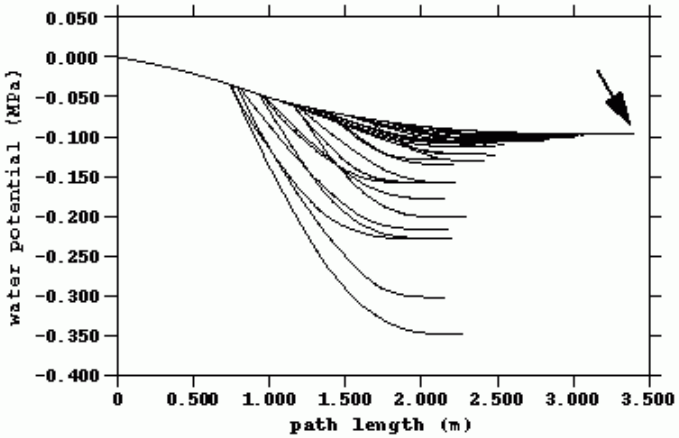
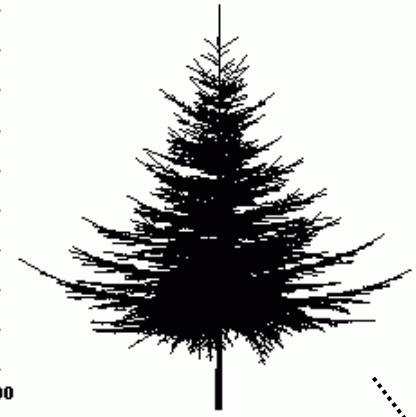
a concept for general representation of dynamics in XL

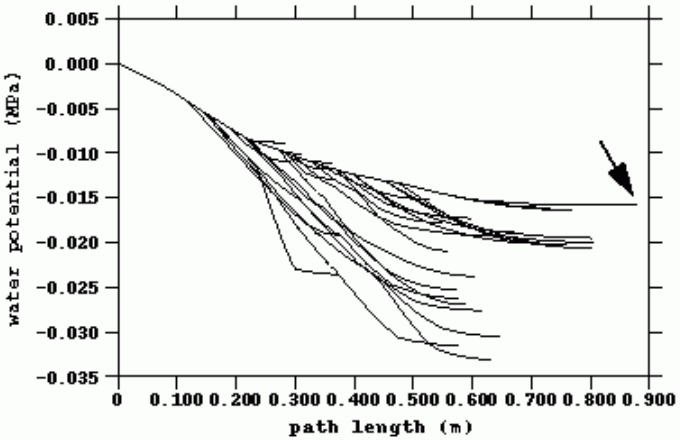
particularly:

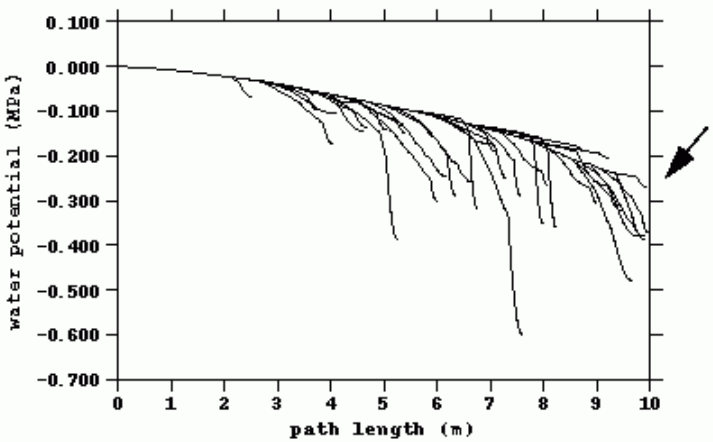
5. Dynamics governed by differential equations

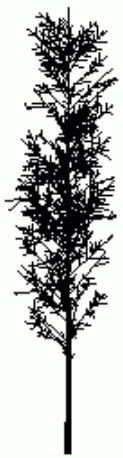
(chemical kinetics is just a special case)











Example: Xylem sap flow model HYDRA (based on differential eq.). Structure has impact on function

(Früh & K. 1999)

Spruce (L-system model)

Spruce (3D measurement)

Thuja (3D measurement)

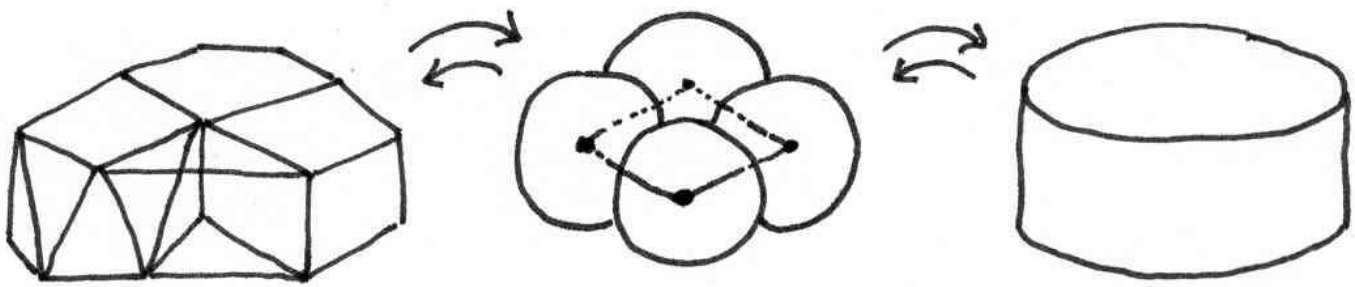
HYDRA until now separated from GROGRA / GroIMP

6. Structure and dynamics of 3D cell assemblies

RGGs are (until now) most often used to produce *tree-like structures*

more general 3D networks and structures should be possible even with the current release of XL

a question: how important is the exact geometry of 2D and 1D boundaries?



7. Rules transforming rules

why this?

Applications:

- Possibility to evolve rules by mutations, again described by rules

- metabolic and regulatory networks define rules for substrate concentrations and/or gene activation

- machine learning
  (to learn means: to change rules, according to meta-rules for learning...)

probably necessary for this purpose:

various unifications

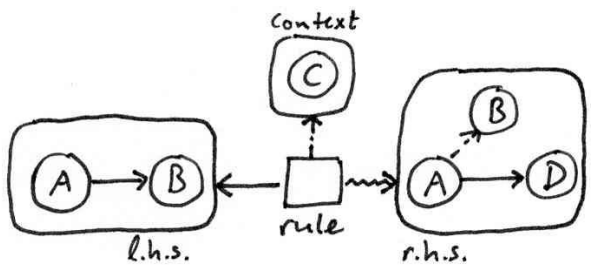
particularly for the concepts of "edge" or "relation":

- graph edges **`-0->`**
- deduced relations **`(>)*`**

already done in XL

- component relation **`a[x]`**
- rule arrows and context delimiters

e.g., rule **`A B, (* C *) ==> A [B] D :`**



- term-building relations

e.g. term **`(x > 2*y) :`**