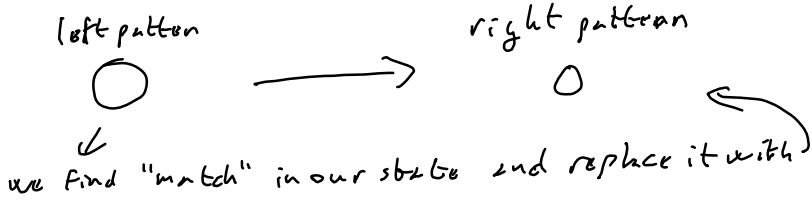
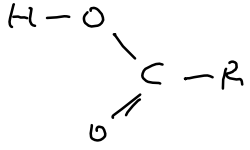
Kappa

Juri Kolčák

Formal Languages

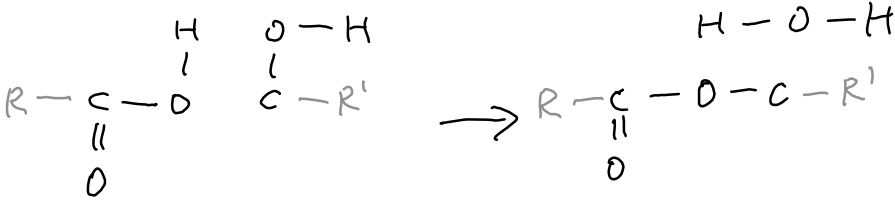
Formal languages are defined on strings, but the same **rule-based transformation** approach can be applied to different structures.





Carboxylic acid

Esterification: $RCOOH + R'COH \rightarrow RCOOCR' + H_2O$



Kappa

Kappa is a relatively young method, although graph transformation itself is much older.

~1973

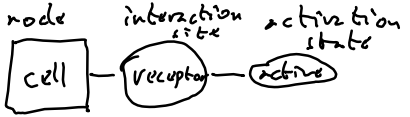
21st cen.

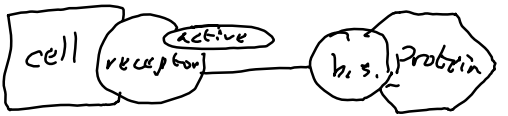
~2010

Applied to a special category of graphs, called **site graphs**.

site graph have nodes = agents / components of the system

each node has interaction sites





each interaction site can have an activation state

Each interaction has a binding state

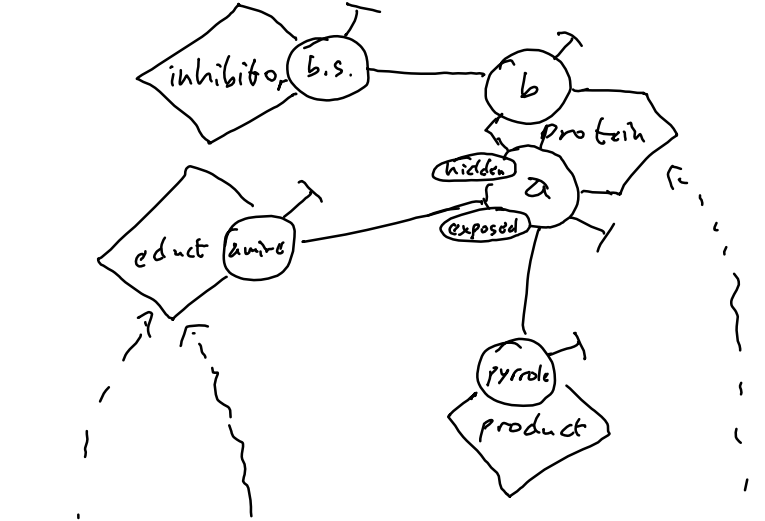
Each interaction site has to have a unique 'name'

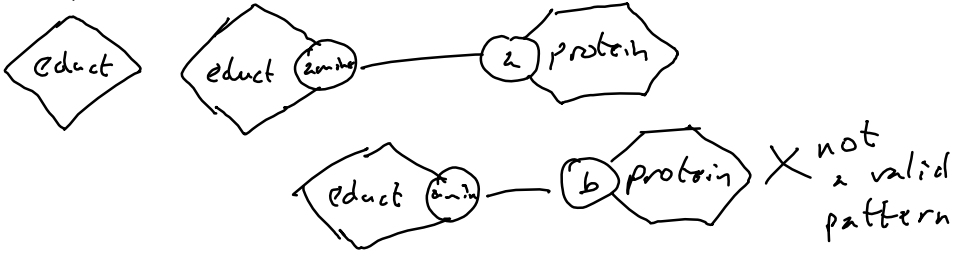
site graphs are rigid

Type Graph

signature / contact map

Effectively the "alphabet" of the model, specifying all types of nodes (agents), their interaction sites, activation and binding states.





Patterns

A pattern is a site graph for which the unique function mapping the pattern into the type graph is a homomorphism.

Patterns can also map into each other, these mappings are called **embeddings**.

The maximal, fully specified, patterns in which all nodes specify all the interaction sites given by the type graph, and each interaction site specifies a binding state as well as an activation state if the type graph specifies any activation states for said site, as called **complexes** and make up the states of the model.