COMPILING MATHEMATICAL FUNCTIONS IN BIOCHEMICAL REACTION NETWORKS

Internship INRIA Lifeware - Julien Bienvenu

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Context – Practical view point

M. Patrick Amar & Sys2diag

- Synthetic vesicles
- Multiple usages (cheap medical testing)

But : Need to figure out real-life CRNs

- Brenda database & BrendaXplorer

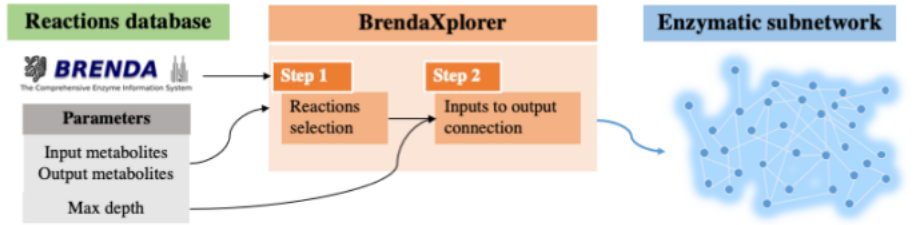


Fig. 2 Database pipeline implemented in BrendaXplorer software to extract concrete chemical reactions, currently used with SiliCell Maker software for implementing logical circuits.

Context – Theoretical viewpoint

- Lifeware & BioCham
- Able through polynomialization to perform the following pipeline :

General objective

Compile general elementary mathematical functions in concrete CRN, by constraining our compilation pipeline to use the ODE terms of a limited set of well-characterized real enzymatic reactions

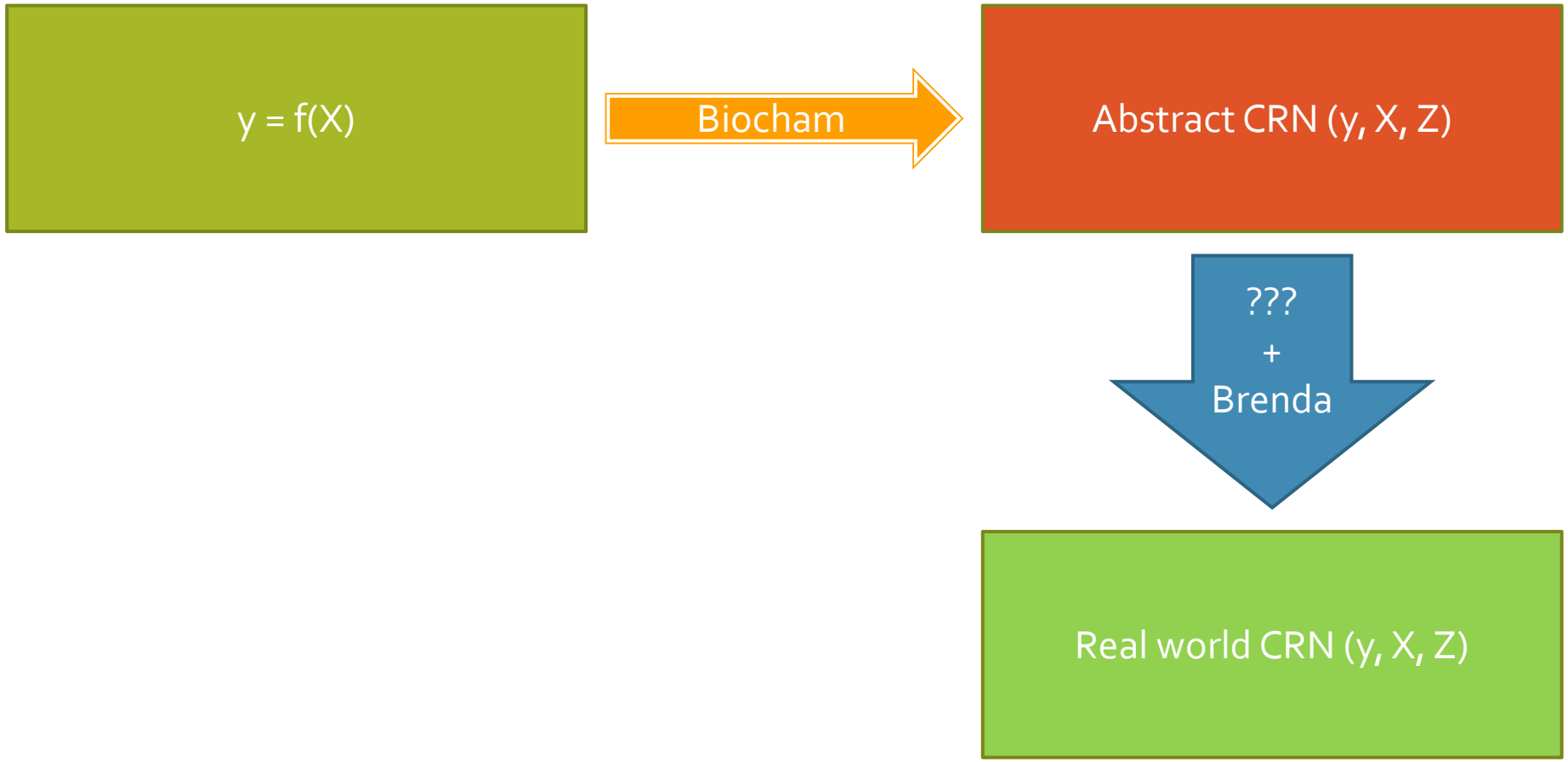
Internship’s objective(s)

Static mapping from the abstract CRN to a concrete CRN (using Brenda as a backend module to Biocham)

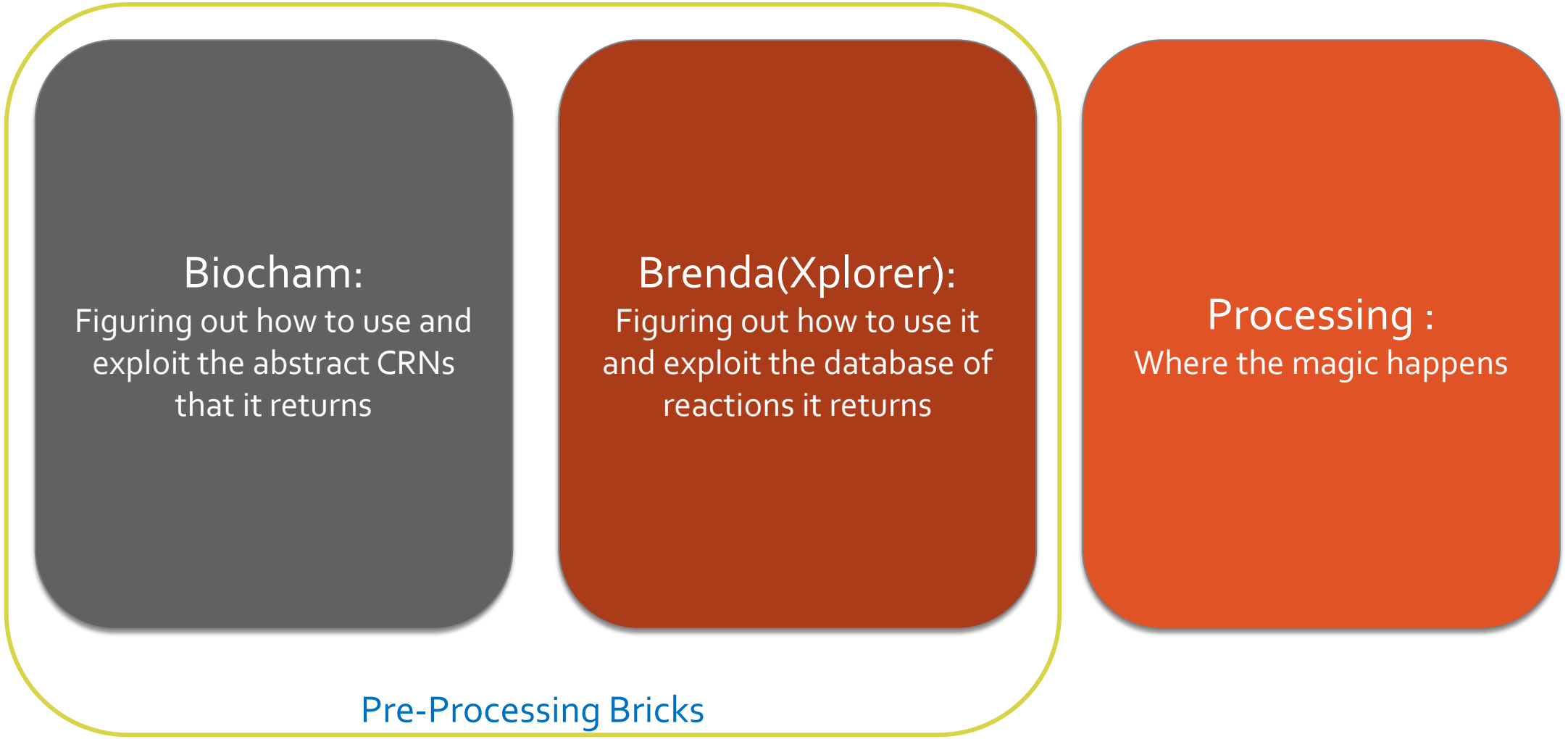
Bonus objective (if there’s time):

Symbolic computation theory of our CRN compilation pipeline in order to constrain it to the limited resources of a reaction catalogue in the early ODE transformation phases

Internship's objective(s)



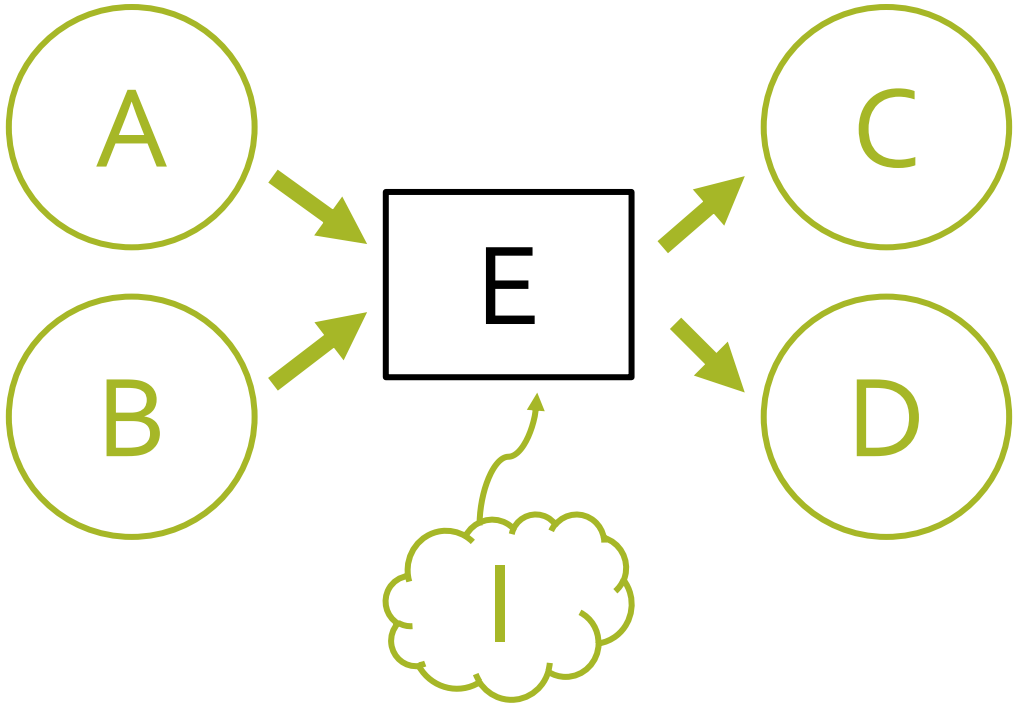
My approach – Dividing in three



My approach – General ideas

- Various objects and classes :
  - Metabolite
  - Reaction
  - Kinetics
  - Environment…
- Loose concept of « matching »
- Abstract CRNs as graphs, with a pre-traversal algorithm
- Dynamic programming to find matching reactions

Some description of CRNs



	E
A	in
B	in
C	out
D	out
I	inhib

Pre-traversal of abstract CRN

- Step 0 : Consider and color as green the predefined metabolites
- Step 1 : Select the enzyme with the most green metabolites and the least red
- Step 2 : Note the enzyme and the new filled metabolites
- Step 3 : Green-light these metabolites for all of their enzymes
- Step 4 : Go back to step 1…

Real-time demo on whiteboard !

Final pipeline

- Pre-traversal optimises the pipeline : aims to show incompatibilities ASAP
- Pre-selecting enzyme candidates for every abstract one in advance matching with it’s abstract kinetic
- Dynamic programming

Key questions (for me)

- How to describe the environment/kinetics ?
- Is the abstract CRN exhaustive ? (Is graph matching enough ?)
- Did I understand the task correctly ?