B2 - Synthesis Pool

B-SYN-200

SBML file parser

Systems Biology Markup Language and parsing

2.0

{EPITECH.}

SBML file parser

binary name: requirement.c, SBMLparser
repository name: SYN_SBMLparser_*$ACADEMICYEAR*
repository rights: ramassage-tek
language: C
compilation: via Makefile, including re, clean and fclean rules

- Your repository must contain the totality of your source files, but no useless files (binary, temp files, obj files,...).
- All the bonus files (including a potential specific Makefile) should be in a directory named *bonus*.
- Error messages have to be written on the error output, and the program should then exit with the 84 error code (0 if there is no error).

Requirement

Write a C file named **requirement.c** containing a function that splits a string into words.
Separators are all non-alphanumeric characters.
The function must return an array, in which each cell contains a string's (representing a word) address.
The last element of the array must be 0, which marks the end of the array.

It should be prototyped the following way:

```
char **my_str_to_word_array_synthesis(char const *str);
```

Only `malloc` and `free` are allowed from the libC.

The rest of the project will not be corrected unless this requirement is fully functional (and rewritten).

The file must be placed at the root of your git repository.
It will be compiled with our main function, and our Makefile (the -I flag being empty).

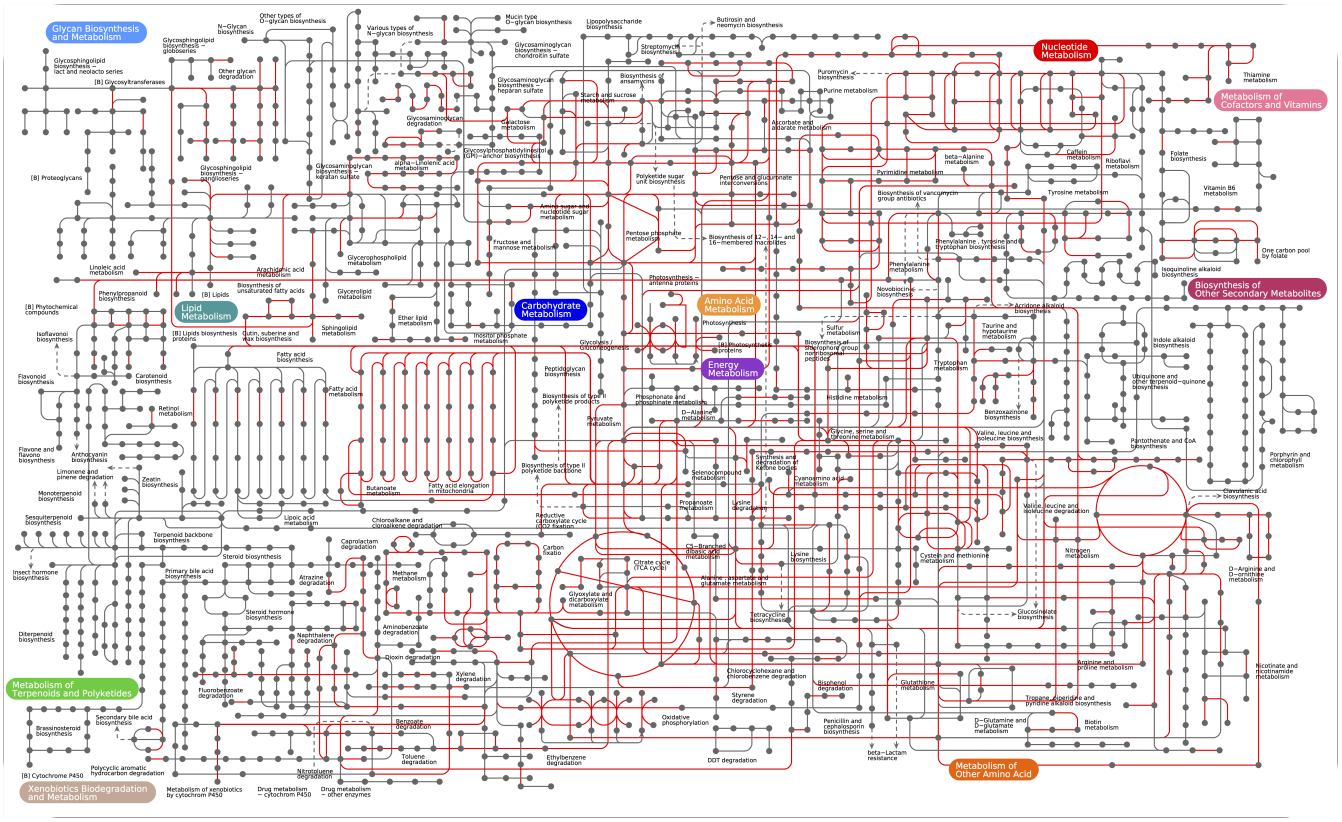
SBML FILE PARSER

Many chemical reactions are responsible for living beings' ability to develop, move, heal, communicate; digestion, for instance, is a chain of chemical reactions.
7439 chemical reactions are present in human beings.

A chemical reaction consists in transforming one or several reactant(s) into one or several product(s). Molecules often have crude names, and are either represented by their chemical formulas or by acronyms; and their reactions are represented by equations such as:

$$C_6H_{12}O_6 + 6O_2 \rightarrow 6CO_2 + 6H_2O + ATP$$
$$ATP + GLCD \rightarrow ADP + G6P$$

Thus, one can demonstrate how a human being functions through the linking of chemical reactions that happen in their cells.
This network is called the metabolic network, and is so complex (as you can see below) that it is a challenge for modern biology.



In order to organize this huge amount of information, a XML-based format, which uses specialized tags for metabolic networks, was created: the **SBML format**.
The main tags are:

1. <compartment> to define the compartment of the reaction,
2. <species> to define a chemical product,
3. <reaction> to define a chemical reaction,
4. <speciesReference> to refer to a previously defined chemical reaction,
5. <listOfCompartments>, <listOfSpecies>, <listOfReactions>, <listOfReactants>, <listOfProducts>, which names are self-exlanatory.

If ever you feel curious, you can download the full specifications here.

As an example, here is *example.sbml*, the SBML file that describes the second aforementioned reaction:

```
<?xml version="1.0" encoding="UTF-8" standalone="no"?>
<sbml xmlns="http://www.sbml.org/sbml/level3/version1/core" level="3" version="1" >
<model name="Homo sapiens Glycolysis" id="Pathway146" >
    <listOfCompartments>
        <compartment name="Homo sapiens, Cell, Cytosol" id="Cytosol"/>
    </listOfCompartments>
    <listOfSpecies>
        <species compartment="Cytosol" name="Adenosine diphosphate" id="Compound1034"
            />
        <species compartment="Cytosol" name="Glucose 6-phosphate" id="Compound1083"/>
        <species compartment="Cytosol" name="Alpha-D-Glucose" id="Compound1851"/>
        <species compartment="Cytosol" name="Adenosine triphosphate" id="Compound414"
            />
    </listOfSpecies>
    <listOfReactions>
        <reaction reversible="false" name="Hexokinase-3" id="Reaction1232" >
            <listOfReactants>
                <speciesReference stoichiometry="1" species="Compound1851"/>
                <speciesReference stoichiometry="1" species="Compound414"/>
            </listOfReactants>
            <listOfProducts>
                <speciesReference stoichiometry="1" species="Compound1083"/>
                <speciesReference stoichiometry="1" species="Compound1034"/>
            </listOfProducts>
        </reaction>
    </listOfReactions>
</model>
</sbml>
```

+ SIMPLE PARSER

Write a program that prints, in alphabetical order, the list of tags and attributes found in the SBML file given as argument.
Each tag and each attribute must be unique.

Don't bother with error management concerning the tags in the SBML file. You'll get only well formatted files.

Your program output has to be strictly identical to the one below.

Terminal

```
~/B-SYN-200> ./SBMLparser example.sbml
compartment
--->id
--->name
model
--->id
--->name
reaction
--->id
--->name
--->reversible
sbml
--->level
--->version
--->xmlns
species
--->compartment
--->id
--->name
speciesReference
--->species
--->stoichiometry
```

+ INFORMATION EXTRACTION

Add the `-i ID` option to your program.

1. If `ID` is the id of a <compartment> tag, the program must print an alphabetical list of id-associated chemical products names on the standard output.
2. If `ID` is the id of a <species> tag, the program must print a quantified and alphabetical list of the chemical reactions ids that consume
a chemical product on the standard output.
3. If `ID` is the id of a <reaction> tag, the program must print an alphabetical list of the reactants, and products of the reaction, on the standard output (identified by their `species`field).
4. Otherwise, the program must print the list of all chemical products.

The *stoichoimetry* tag gives the quantity of consumed chemical products.

Your program output has to be strictly identical to the one below.

```
Terminal
~/B-SYN-200> ./SBMLparser example.sbml -i Cytosol
List of species in compartment Cytosol
--->Adenosine diphosphate
--->Adenosine triphosphate
--->Alpha-D-Glucose
--->Glucose 6-phosphate
```

```
Terminal
~/B-SYN-200> ./SBMLparser example.sbml -i ChuckNorris
List of species
--->Adenosine diphosphate
--->Adenosine triphosphate
--->Alpha-D-Glucose
--->Glucose 6-phosphate
```

```
Terminal
~/B-SYN-200> ./SBMLparser example.sbml -i Compound414
List of reactions consuming species Compound414 (quantities)
--->Reaction1232 (1)
```

```
Terminal
~/B-SYN-200> ./SBMLparser example.sbml -i Reaction1232
List of reactants of reaction Reaction1232
--->Compound1851
--->Compound414
List of products of reaction Reaction1232
--->Compound1034
--->Compound1083
```

Add the `-e` option to print the equation of the reaction, if ID is a reaction id.

If the reaction is reversible, the arrow is to be represented by "<->".

Your program output has to be strictly identical to the one below.

```
Terminal
~/B-SYN-200> ./SBMLparser example.smbl -i Reaction1232 -e
1 Compound1851 + 1 Compound414 -> 1 Compound1034 + 1 Compound1083
```

+ SBML TO JSON

Add the `-json` option to convert the SBML file into JSON.

Tags and attibutes taken into account will be the one in the SBML file given in the previous example, and only these ones.

If the `-i` option must be filled in, and:

1. if the id is a compartment, only this compartment, and the chemical products and reactions referring to it, must be displayed,
2. if the id is a chemical product, only this product, and the compartments and reactions referring to it, must be displayed,
3. if the id is a reaction, only this reaction, and the chemical products and compartments referring to it, must be displayed,
4. otherwise, the `-json` option is ignored.

Terminal

```
~/B-SYN-200> ./SBMLparser -h
USAGE
      ./SBMLparser SBMLfile [-i ID [-e]] [-json]

DESCRIPTION
      SBMLfile    SBML file
      -i ID       id of the compartment, reaction or product to be extracted
                  (ignored if uncorrect)
      -e          print the equation if a reaction ID is given as argument
                  (ignored otherwise)
      -json       transform the file into a JSON file
```

Terminal

```
~/B-SYN-200> ./SBMLparser example.sbml -i Compound414 -json
{
"listOfCompartments": [
    {
      "id": "Cytosol",
      "name": "Homo sapiens, Cell, Cytosol"
    }
],
"listOfSpecies": [
    {
      "compartment": "Cytosol",
      "id": "Compound414",
      "name": "Adenosine triphosphate"
    }
],
"listOfReactions": [
    {
      "id": "Reaction1232",
      "name": "Hexokinase-3",
      "reversible": "false"
    }
]
}
```

Terminal

```
~/B-SYN-200> ./SBMLparser example.sbml -i Reaction1232 -json
{
"listOfReactants": [
    {
      "species": "Compound1851",
      "stoichiometry": "1"
    },
    {
      "species": "Compound414",
      "stoichiometry": "1"
    }
],
"listOfProducts": [
    {
      "species": "Compound1083",
      "stoichiometry": "1"
    },
    {
      "species": "Compound1034",
      "stoichiometry": "1"
    }
]
}
```