BIOINFORMÁTICA

Asignatura 400CIS016
Doctorado en Ingeniería

Pontificia Universidad JAVERIANA Cali

Wednesday March 01, 2017 (2:00-6:00PM)
FINAL PROJECT: Please, elaborate and send to dphermith@javerianacali.edu.co a report in format "pdf" including the development of the following formulations:

1. Compare the time course of the model MMexact.bngl with the results of the model MMapprox.bngl. Both inputs can be found at http://bionetgen.org/index.php/MMexact.bngl and http://bionetgen.org/index.php/MMapprox.bngl, respectively (Hint: Elaborate a table by including different values for the rate constants and the reactants concentration).

2. In the model MMapprox.bngl to directly compare the rates of substrate conversion between this one and the exact model (MMexact.bngl), try adding the following function:

```
ES_eff() E0*Su/(Km + Su) #effective amount of ES complex used to compute the rate of the MM reaction
```

Support your explanation with the graphical output of the simulation.

3. In Biocham, build and simulate the Brusselator model. It is a type of an oscillating reaction system (i.e., an autocatalytic reaction system) based on the Belousov-Zhabotinsky reaction [Singh 2008, Kang 2005] in which a molecular species acts to increase the rate of its producing reaction. It has been quite well studied because of its theoretical simplicity, while it retains the functional form of more complex reaction networks. It can be used an arbitrary set of rate constants.

A reaction scheme for the Brusselator (i.e., an autocatalytic reaction system)
R_1: $A \rightarrow X$
R_2: $B + X \rightarrow Y + D$
R_3: $2X + Y \rightarrow 3X$
R_4: $X \rightarrow C$
A, B, D, C, X, Y: are molecular species
X, Y: are the autocatalytic species
R_1: produces objects of type X
R_2: consumes X and produces objects of type Y
R_3: uses a copy of Y for increasing the number of X
R_4: allows the system to consume the objects X

Support your observations with the graphical output of the simulation. Try to use the three

semantics available. Besides, try to perform the automatic checking of the following CTL properties for some of the molecular species in the system (Please, provide snapshots to support your query):

1. Reachability: where reachable(P) stands for EF(P).
2. Steady states: where steady(P) stands for EG(P).
3. Stable states: where stable(P) stands for AG(P).

4. Read and analyze the following statement:

> *"Biological organisms are complex because they are characterized by hierarchies of self-assembled networks. Networks of interacting molecules at the level of the cell, interacting molecules and cells at the level of tissues, interacting organs at the level of the organisms, and interacting organisms at the level of ecosystems. These interactions/networks are well organized in space and time, normally, they are non-linear and there are a large number of them".*

Provide and reference at least three arguments to support this statement based on the readings assigned in the course.

References:

[Singh 2008] Rajeev Singh. Brusselator as a reaction-diffusion system. Master's thesis, The Institute of Mathematical Sciences, Chennai, May 2008.

[Kang 2005] Hunseok Kang and Yakov Pesin. Dynamics of a Discrete Brusselator Model: Escape to Infinity and Julia Set. Milan Journal of Mathematics, vol. 73, no. 1, pages 1–17, 2005.