**Introduction to SimBiology**

What is SimBiology?

The MATLAB package houses a package called SimBiology that permits the development of models of biological systems. As a graphical, intuitive interface, it allows the establishment of models that would otherwise require an awareness of the differential equations of the system being examined.

What are projects and libraries with SimBiology?

Within the SimBiology environment, models are built and its analysis workflow managed through the use of SimBiology projects and SimBiology libraries. Specifically, projects are used to enable models to be created and to analyses associated tasks and data into one package. The development of models within projects is assisted by the presence of libraries that house information regarding units, kinetic laws and plot types.

Gene Regulation Model

The model under consideration is an example of simple gene regulation, in which the protein product of translation forms a negative feedback loop on its own transcription. This model can undergo subsequent rounds of refinement in order to make it more complex by additional biomolecules such as enzymes and nucleotides. In this example, the regulatory mechanism under operation within this gene expression model does not include the important contributions of RNA polymerase and any cofactors. This gene expression model is an example by which binding of the protein product to a region of DNA represses transcription.

![Gene Regulation Model Diagram]

*Figure 1* Gene expression model of a protein that negatively regulates its own production. The reactions described within this model occur within distinct organelles within the cell, e.g. the transcription of DNA into primary mRNA transcript occurs within the nucleus.
Protocol for modelling with SimBiology

1. Launch SimBiology by typing “simbiology” into the MATLAB command prompt.
2. In order to create a new model, click on the ‘Add Model’ tab and subsequently the “Create a blank model”.
3. Species and reactions can be added to the model by using the Block Library Browser to the lower left.
4. Configure the kinetics of the reactions with the help of the window titled “ModelBuilding: Reaction Properties”.
5. Input the initial conditions
6. The model can be simulated in a time-course in order to establish changes in mRNA concentration over time. Selecting the “Simulate Model” within the “Add” menu of the Project Explorer window can do this.
7. The parameters of the model can be modified to observe changes.

More Options

Diagram
Alter the direction of a reaction by specifying the reactant/product or both
Indicate whether a reaction is reversible
Restrict species to particular compartments of the cell

Compartments / species
The initial concentrations can be specified in each compartment.

Reactions
A variety of reaction kinetics are available.

Rules
Algebraic rules can be applied to establish the concentration of a species or a rate constant

Events
An event can be specified by a time component or by the concentration of a species, at which point a rate constant or a species concentration will change.

Data Logging
The Data Logging Tab provides the option to select the variables to be displayed.

Links
