User guide to PNK 2e

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This is the manual for PNK 2e, a software developed using the Petri Net Kernel (PNK) version 2.2. The Petri Net Kernel is a framework for the development of Petri Net tools. It was developed at the Humboldt University of Berlin, Germany. Its extended version, PNK 2e, was developed by Ole Schulz-Trieglaff, during his M.Sc. dissertation at the University of Edinburgh, UK. PNK 2e features Stochastic Petri Nets, a modelling formalism that stems from Computer Science. Stochastic Petri Nets (SPNs) are closely related to Markov Jump Processes. Their behaviour can be simulated using the Gillespie Algorithm and its improved vesions (Gibson-Bruck, Tau Leap).

PNK 2e extends the PNK by features for the modelling of biological processes. PNK 2e means "extended Petri Net Kernel version 2". The software is able to create a Petri Net representation of a model described in SBML (Systems Biology Workbench Language). The net is drawn by using a simple algorithm implemented by Alexander Gruenewald, Humboldt University of Berlin. The dynamic behaviour of the Petri Net can be simulated using the Systems Biology Workbench. In order to achieve this, PNK 2e translates the net back into its SBML description and passes this description automatically to the Workbench. Alternatively, a Petri Net can be created using the graphical editor of the Kernel.

Licence Agreement

Quick start

This is a brief introduction to PNK 2e. The software requires the Java version $\geq$ 1.2.2. The archive *PNK2e.zip* can be downloaded from `www.inf.fu-berlin.de/ trieglaf/PNK2e` and contains all necessary files. The Systems Biology Workbench is required to perform the simulation of the Petri Net and is available at `http://sbw.kgi.edu/`.

Download and run the software

If the archive *PNK2e.zip* is extracted, a new directory `PNK2e` should be created in the current directory. This directory contains several libraries in *.jar* format, the file *PNK2e.jar* which is the program itself and several subdirectories:

- sampleNets - contains some netexamples
- netTypeSpecifications - contains examples for a net's specification
- toolSpecification - contains some toolspecification examples

If anything goes wrong, first check if you have the correct version of Java installed by executing
`java -version`. Then try to find out if all necessary libraries are contained in the same directory as the *.jar* file. PNk 2e needs at least the libraries *jaxp.jar*, *crimson.jar*, *SBWcore.jar* and *SBMLreader.jar*. The remaining libraries are needed for the translation of Petri Nets into CMDL only.

How to open, edit and save a Petri Net

The software can be started by double-clicking on the file *PNK2e.jar* (Windows) or by executing `java -jar PNK2e.jar` (Linux and other operating systems). The main menu of PNK 2e should appear. By clicking on the *File* menu, the user can open a file and load the net into the Kernel (see screenshot 1). The editor is opened automatically and displays the net.

Alternatively, the user can select *New* in the menu *Open* of the main menu to create a new Petri Net. PNK 2e can edit Stochastic Petri Nets, Biological Nets (SPNs with simplifactions for biological reactions) and Generalized Stochastic Nets (SPNs with inhibitor arcs and immediate transitions). Depending on this choice, the main menu changes to the editor menu. This menu offers the user the possibility to draw places and transitions by simply choosing the type of node to be drawn and by clicking into the editor pane. Arcs can be drawn by first clicking on the source node and then on the target node. PNK 2e also contains a function to automatically arrange a net. This function is called *DoNetLayout* and is available in the main menu.

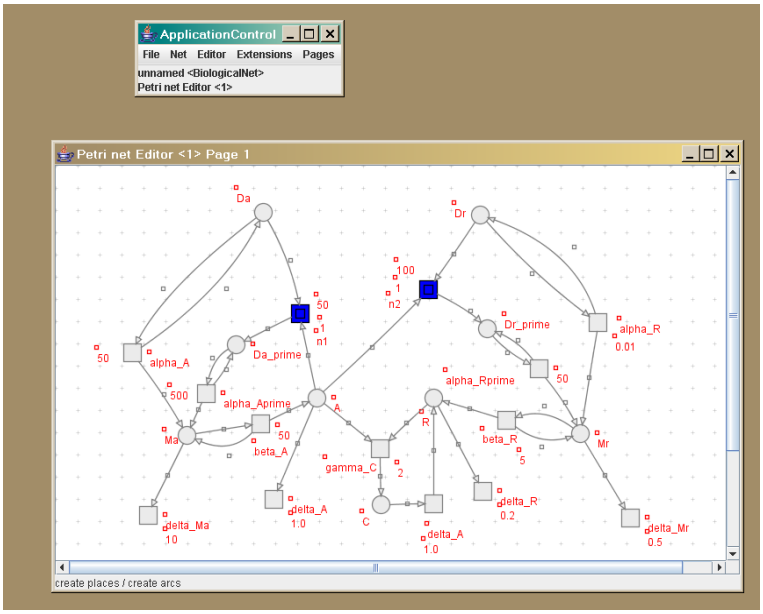

Figure 1: *PNK 2e after loading the SPN representation of a genetic oscillator.*

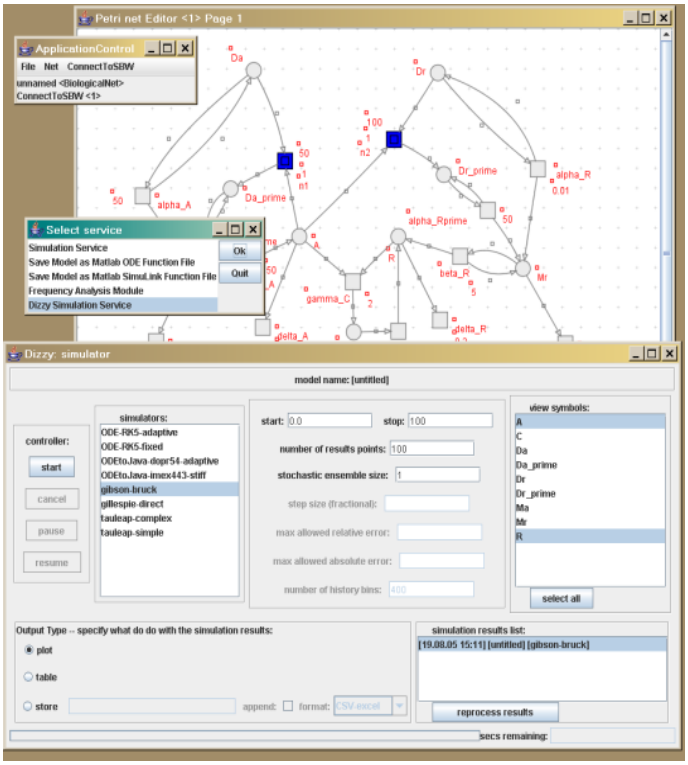

Figure 2: *The simulation interface of PNK 2e.*

Simulating a net

PNK 2e can simulate a Stochastic Net. This simulation is conducted in form of a "token game", that is a transition that is executed is coloured for some milliseconds and the flow of the token through the net is visualised. This simulation is available in the main menu under *stochastic simulation*.

This simulation is the correct way to simulate the net and gives a good idea of its dynamics. However, it is not well suited for large nets since it is very slow. Furthermore, data of the simulation run is not collected. If a more detailed analysis of the simulation is required, the user can choose the entry *ConnectToSBW* in the main menu. PNK2e then opens a window with a list of all services in the Systems Biology Workbench that are available on this computer. For a description of the SBW and on how to install new modules and services, have a look at the manual of the SBW which is available at `http://sbw.kgi.edu/`. We recommend to install the simulator *Dizzy* in addition to the workbench because this software offers several simulation algorithms, stochastic and deterministic, and works very well with PNK 2e. But every simulation software is compatible to the Systems Biology Workbench and implements the Gillespie algorithm or one of its improved versions can be used.

If Dizzy is installed, the list of SBW services should contain an entry *Dizzy simulation service*. After clicking on this entry, the Dizzy simulation window opens (see screenshot 2). The window contains a list with all available simulation algorithms. Start and end time of the simulation can be chosen. In case of a stochastic simulation, the user can also decide to average the result over several runs. If a deterministic simulation is chosen, the user has also decide about step size and maximum relative and absolute error.

The simulation is started by clicking on the *Start* button on the left side of the simulation windew. The simulation can be paused by clicking on *Pause* and resumed by clicking on *Resume*. At the end of the simulation, results can be plotted or written to a file.