NoPain – Meeting

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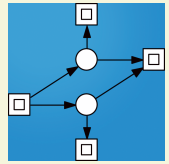
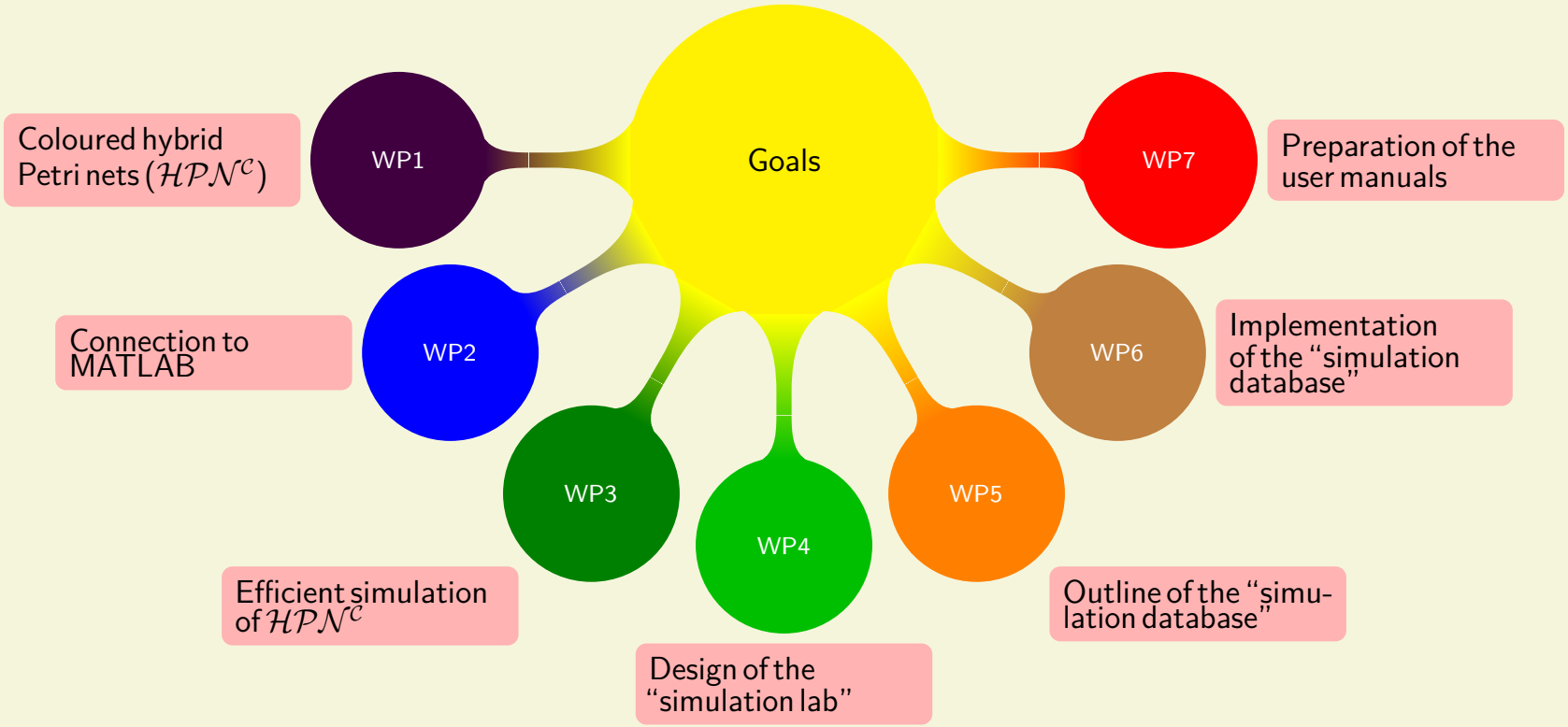
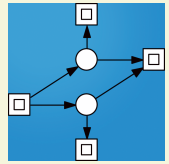
Work Packages





WP2



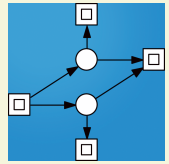
Connection to MATLAB

a. Predecessor WPs: BTU-WP1

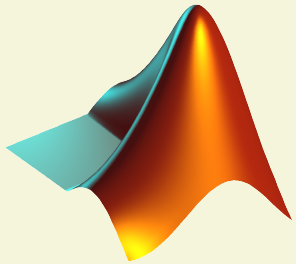
b. Successor WPs: BTU-WP7

- Connection of the MATLAB software package to the hybrid Petri nets as well as to relevant net classes
  1. Export the net structure in MATLAB format
  2. Direct connection from Snoopy to MATLAB through its API, e.g. call MATLAB functions from within Snoopy

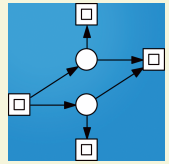
MATLAB



- MATLAB is a high-level language and interactive environment for numerical computation, visualization, and programming.
- You can use MATLAB for a range of applications, including signal processing and communications, image and video processing, control systems, test and measurement, computational finance, and computational biology.
- Commercial product of MathWorks.

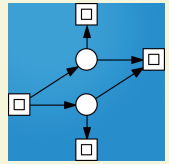


Octave



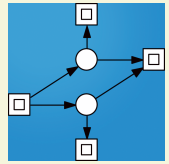
- Octave is a high-level interpreted language, primarily intended for numerical computations.
- It provides capabilities for the numerical solution of linear and nonlinear problems, and for performing other numerical experiments.
- It also provides extensive graphics capabilities for data visualization and manipulation.
- The Octave language is quite similar to MATLAB so that most programs are easily portable.
- Octave is distributed under the terms of the GNU General Public License.

Scilab



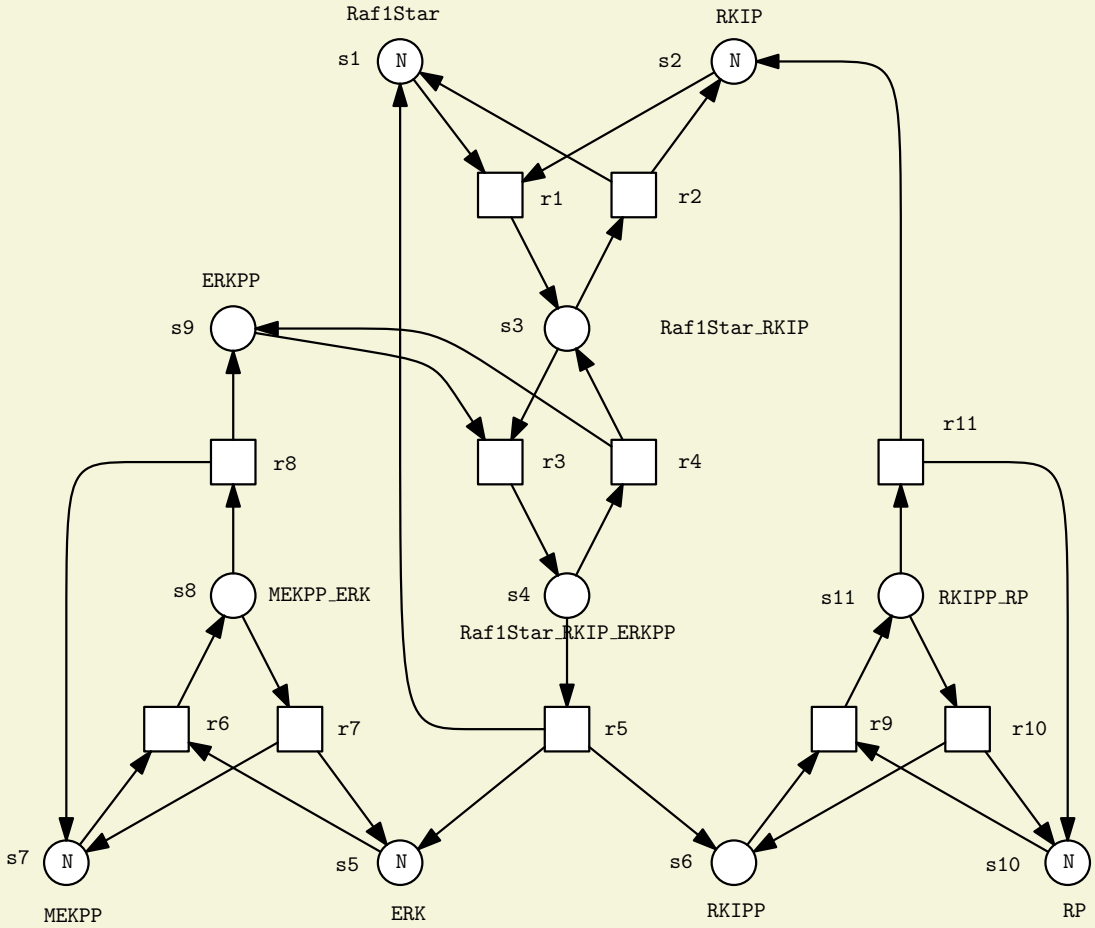
- Scilab is free and open source software for numerical computation providing a powerful computing environment for engineering and scientific applications.
- It has a high level programming language allowing access to advanced data structures, 2-D and 3-D graphical functions.
- A large number of functionalities is included in Scilab: control, simulation, optimization, signal processing..., and Xcos, the hybrid dynamic systems modeller and simulator is provided with the platform.
- As the syntax of Scilab is similar to MATLAB, Scilab includes a source code translator for assisting the conversion of code from MATLAB to Scilab.

Example

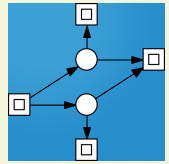


RKIP inhibited ERK Pathway

RKIP/MEK-ERK signalling pathway [wolkenhauer 2003], [Calder 2005]



Example

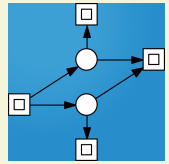


RKIP inhibited ERK Pathway – MATLAB code

```
%% Petri net
pn.Name = 'erk_N'

% place vector
pn.P = {'Raf1Star', 'RKIP', 'Raf1Star_RKIP', 'ERKPP', 'MEKPP_ERK', 'Raf1Star_RKIP_ERKPP',
        'RKIPP_RP', 'MEKPP', 'ERK', 'RKIPP', 'RP'};
% marking vector
pn.m0 = [1, 1, 0, 0, 0, 0, 0, 1, 1, 0, 1];
% transition vector
pn.T = {'r1', 'r2', 'r3', 'r4', 'r5', 'r6', 'r7', 'r8', 'r9', 'r10', 'r11'};
pn.C = {0.53, 0.0072, 0.625, 0.00245, 0.0315, 0.8, 0.0075, 0.071, 0.92, 0.00122, 0.87};
```

Example



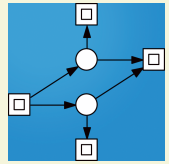
RKIP inhibited ERK Pathway – MATLAB code

```
pn.PreArcs = [
1,0,0,0,0,0,0,0,0,0,0;
1,0,0,0,0,0,0,0,0,0,0;
0,1,1,0,0,0,0,0,0,0,0;
0,0,1,0,0,0,0,0,0,0,0;
0,0,0,0,0,0,1,1,0,0,0;
0,0,0,1,1,0,0,0,0,0,0;
0,0,0,0,0,0,0,0,0,1,1;
0,0,0,0,0,1,0,0,0,0,0;
0,0,0,0,0,1,0,0,0,0,0;
0,0,0,0,0,0,0,0,1,0,0;
0,0,0,0,0,0,0,0,1,0,0;
];
```

```
pn.PostArcs = [
0,1,0,0,1,0,0,0,0,0,0;
0,1,0,0,0,0,0,0,0,0,1;
1,0,0,1,0,0,0,0,0,0,0;
0,0,0,1,0,0,0,1,0,0,0;
0,0,0,0,0,1,0,0,0,0,0;
0,0,1,0,0,0,0,0,0,0,0;
0,0,0,0,0,0,0,0,1,0,0;
0,0,0,0,0,0,1,1,0,0,0;
0,0,0,0,1,0,1,0,0,0,0;
0,0,0,0,1,0,0,0,0,1,0;
0,0,0,0,0,0,0,0,0,1,1;
];
```

```
% stochiometric matrix (standard edges with weights)
pn.S = pn.Post - pn.Pre;
```

Example



RKIP inhibited ERK Pathway – MATLAB code

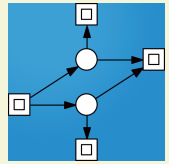
```
pn.ReadArcs = [
0,0,0,0,0,0,0,0,0,0,0,0;
0,0,0,0,0,0,0,0,0,0,0,0;
0,0,0,0,0,0,0,0,0,0,0,0;
0,0,0,0,0,0,0,0,0,0,0,0;
0,0,0,0,0,0,0,0,0,0,0,0;
0,0,0,0,0,0,0,0,0,0,0,0;
0,0,0,0,0,0,0,0,0,0,0,0;
0,0,0,0,0,0,0,0,0,0,0,0;
0,0,0,0,0,0,0,0,0,0,0,0;
0,0,0,0,0,0,0,0,0,0,0,0;
0,0,0,0,0,0,0,0,0,0,0,0;
];
```

```
pn.InhibitorArcs = [
0,0,0,0,0,0,0,0,0,0,0,0;
0,0,0,0,0,0,0,0,0,0,0,0;
0,0,0,0,0,0,0,0,0,0,0,0;
0,0,0,0,0,0,0,0,0,0,0,0;
0,0,0,0,0,0,0,0,0,0,0,0;
0,0,0,0,0,0,0,0,0,0,0,0;
0,0,0,0,0,0,0,0,0,0,0,0;
0,0,0,0,0,0,0,0,0,0,0,0;
0,0,0,0,0,0,0,0,0,0,0,0;
0,0,0,0,0,0,0,0,0,0,0,0;
0,0,0,0,0,0,0,0,0,0,0,0;
];
```

```
pn.ResetArcs = [
0,0,0,0,0,0,0,0,0,0,0,0;
0,0,0,0,0,0,0,0,0,0,0,0;
0,0,0,0,0,0,0,0,0,0,0,0;
0,0,0,0,0,0,0,0,0,0,0,0;
0,0,0,0,0,0,0,0,0,0,0,0;
0,0,0,0,0,0,0,0,0,0,0,0;
0,0,0,0,0,0,0,0,0,0,0,0;
0,0,0,0,0,0,0,0,0,0,0,0;
0,0,0,0,0,0,0,0,0,0,0,0;
0,0,0,0,0,0,0,0,0,0,0,0;
0,0,0,0,0,0,0,0,0,0,0,0;
];
```

```
pn.ModifierArcs = [
0,0,0,0,0,0,0,0,0,0,0,0;
0,0,0,0,0,0,0,0,0,0,0,0;
0,0,0,0,0,0,0,0,0,0,0,0;
0,0,0,0,0,0,0,0,0,0,0,0;
0,0,0,0,0,0,0,0,0,0,0,0;
0,0,0,0,0,0,0,0,0,0,0,0;
0,0,0,0,0,0,0,0,0,0,0,0;
0,0,0,0,0,0,0,0,0,0,0,0;
0,0,0,0,0,0,0,0,0,0,0,0;
0,0,0,0,0,0,0,0,0,0,0,0;
0,0,0,0,0,0,0,0,0,0,0,0;
];
```

Example

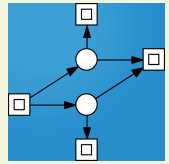


RKIP inhibited ERK Pathway – MATLAB code

```
% Simulation parameter
pn.t_start = 0; %start time
pn.t_end = 100; %end time
pn.t_step = 1; %sample interval for gathering data (optimal, only for SPN)
pn.runs = 1; % number of simulation runs (optimal, only for SPN)

%CPN2Matlab(pn);
SPN2Matlab(pn);
```

MATLAB Code



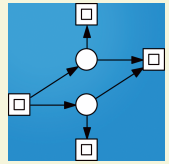
Working

- Export net structure including places, transitions and arcs (including special arc types).
- Export of rate constants for stochastic transitions
- Use of built-in sparse matrix representation to save memory.
- Run stochastic simulation assuming mass-action kinetics.

Not working

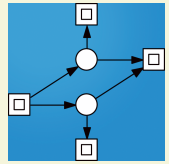
- Non-stochastic transition types (immediate, deterministic and scheduled transitions).
- User-defined rate functions.

Milestones



	2013				2014				2015			
	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
WP1		M1										
WP2				M2								
WP3						M3						
WP4								M4				
WP5								M4				
WP6												M5
WP7												M6

Next steps...

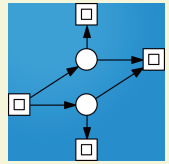


Connection to MATLAB

- Reaching 2nd milestone.

Efficient simulation of $\mathcal{HPN}^{\mathcal{C}}$

- Examination of the Petri net models with regard to parallelisation potential.
- Investigation of optimisation possibilities and performance comparisons with alternative tools, i.e. MATLAB, Cain...



Thank you for your attention!