

CellDesigner 4.0beta

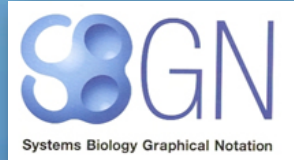
Akira Funahashi
Keio University
The Systems Biology Institute
30th Jan. 2008



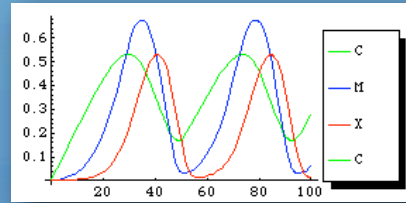
CellDesigner



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= CellDesigner

The screenshot displays the CellDesigner interface with the following components:

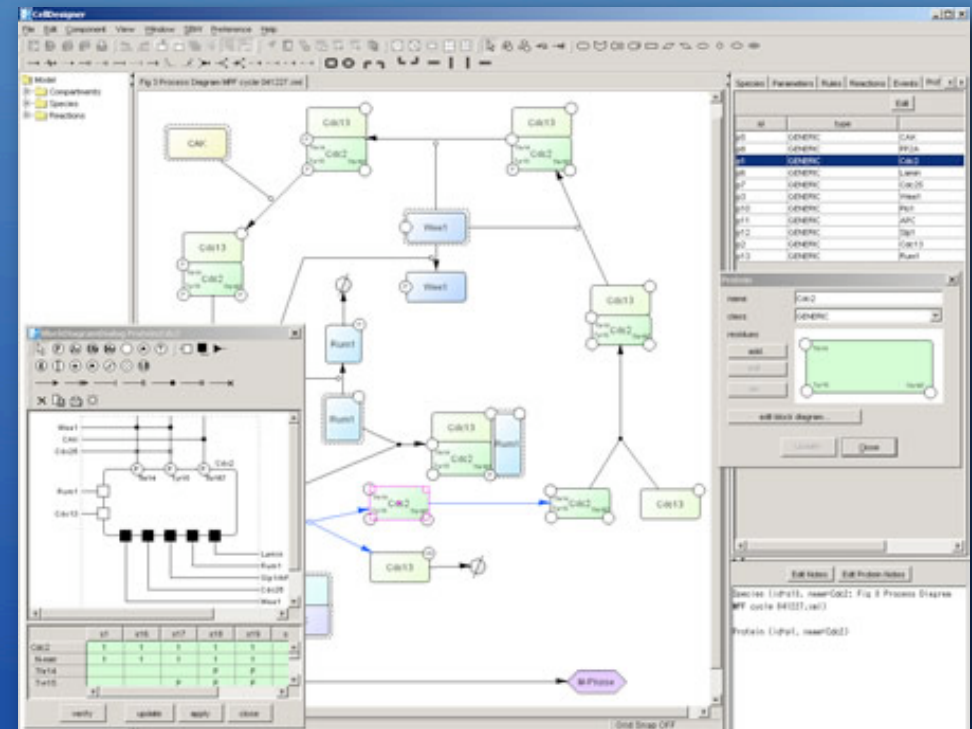
- Species List:**

id	type	name
p5	GENERIC	CAK
p8	GENERIC	PP2A
p1	GENERIC	Cdc2
p6	GENERIC	Lamin
p7	GENERIC	Cdc25
p3	GENERIC	Wee1
p10	GENERIC	Plo1
p11	GENERIC	APC
p12	GENERIC	Slp1
p2	GENERIC	Cdc13
p13	GENERIC	Rum1
- Protein Detail Panel:**

name	class
Cdc2	GENERIC
- Simulation Graph:** Shows concentration vs time for various species, with a y-axis from 0.00 to 306.82 and an x-axis from 0 to 1000.00.
- Network Diagram:** A complex biochemical network with nodes like CAK, Cdc13, Cdc2, Wee1, Rum1, APC, and Slp1, connected by regulatory interactions.

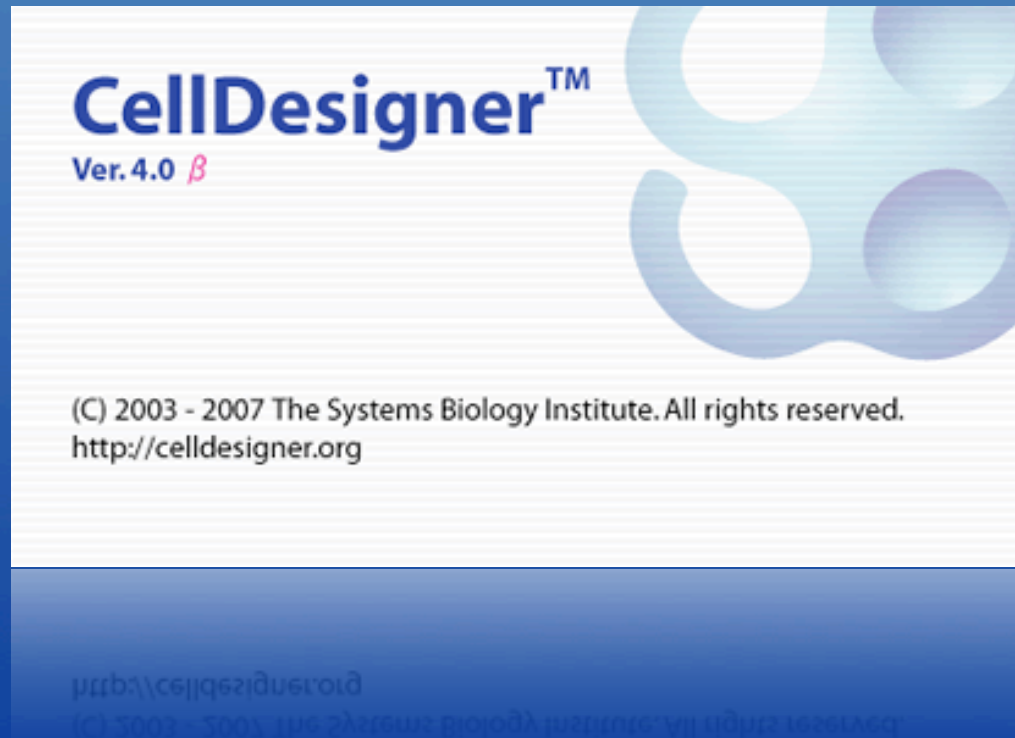
Modeling tool for biochemical and gene-regulatory network

- SBML support
- Graphical notation (Process diagram)
- Built-in simulator (SBML ODE Solver)
- Integrate with Analysis tool, other simulators through SBW
- Database connection
- Export to PDF, PNG, etc.
- Freely available
- Supported Environment
 - Windows (2000 or later)
 - Mac OS X
 - Linux



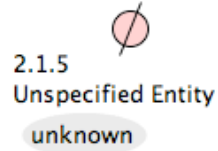
CellDesigner 4.0 (beta)

- Graphical Notation (SBGN Level-1 draft)
- Usability
- Plugin development framework
- Integrate with other tools / services

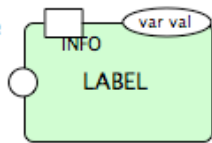


Tag...

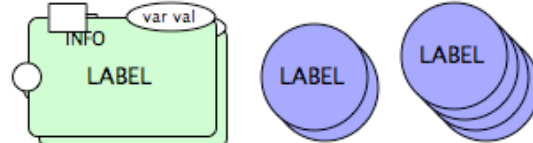
2.1.4 Source-Sink



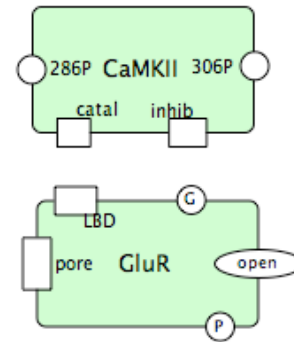
2.1.7 Macromolecule



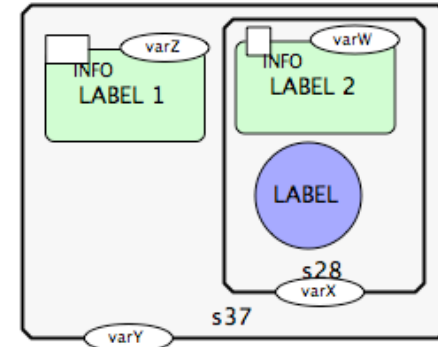
2.1.8 Multimer



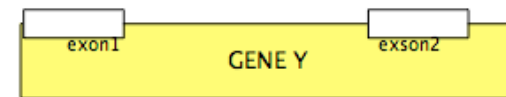
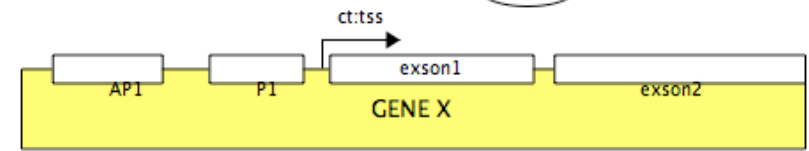
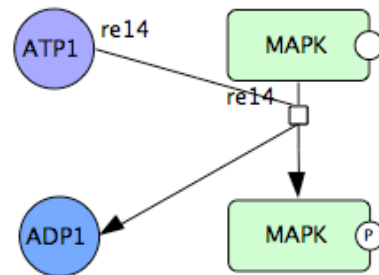
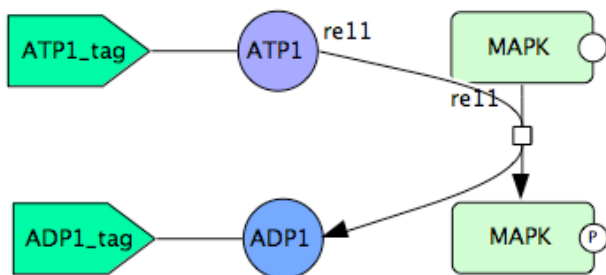
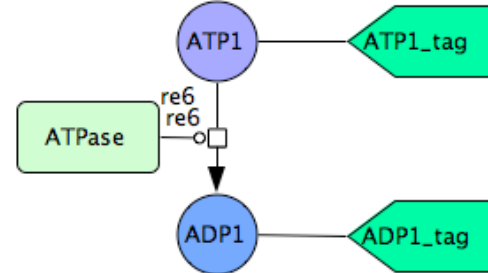
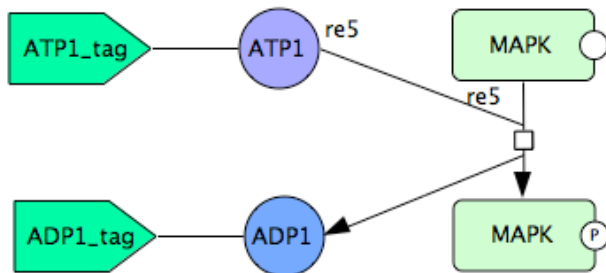
2.1.10 Example of complex SENS



2.2.1 Complex



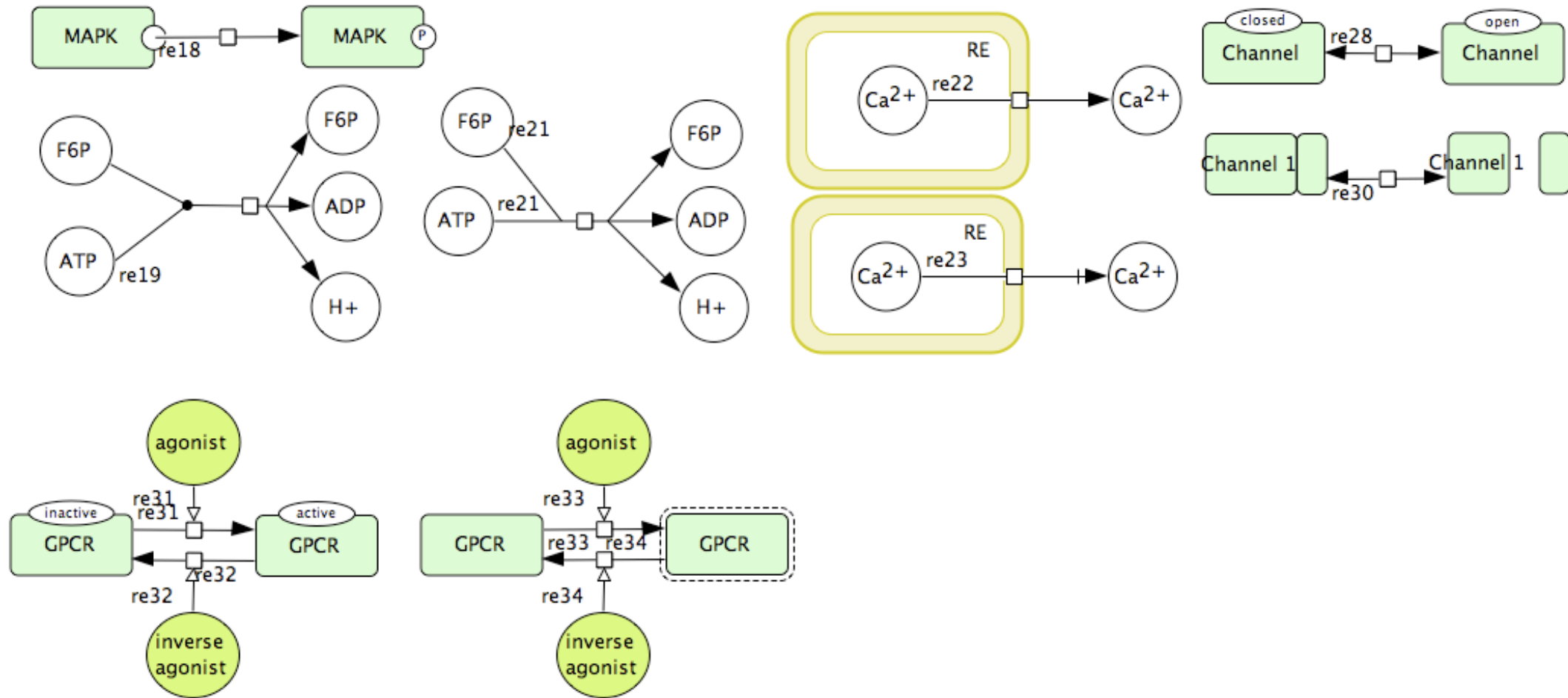
2.1.3 Tag



2.3.1 Transition

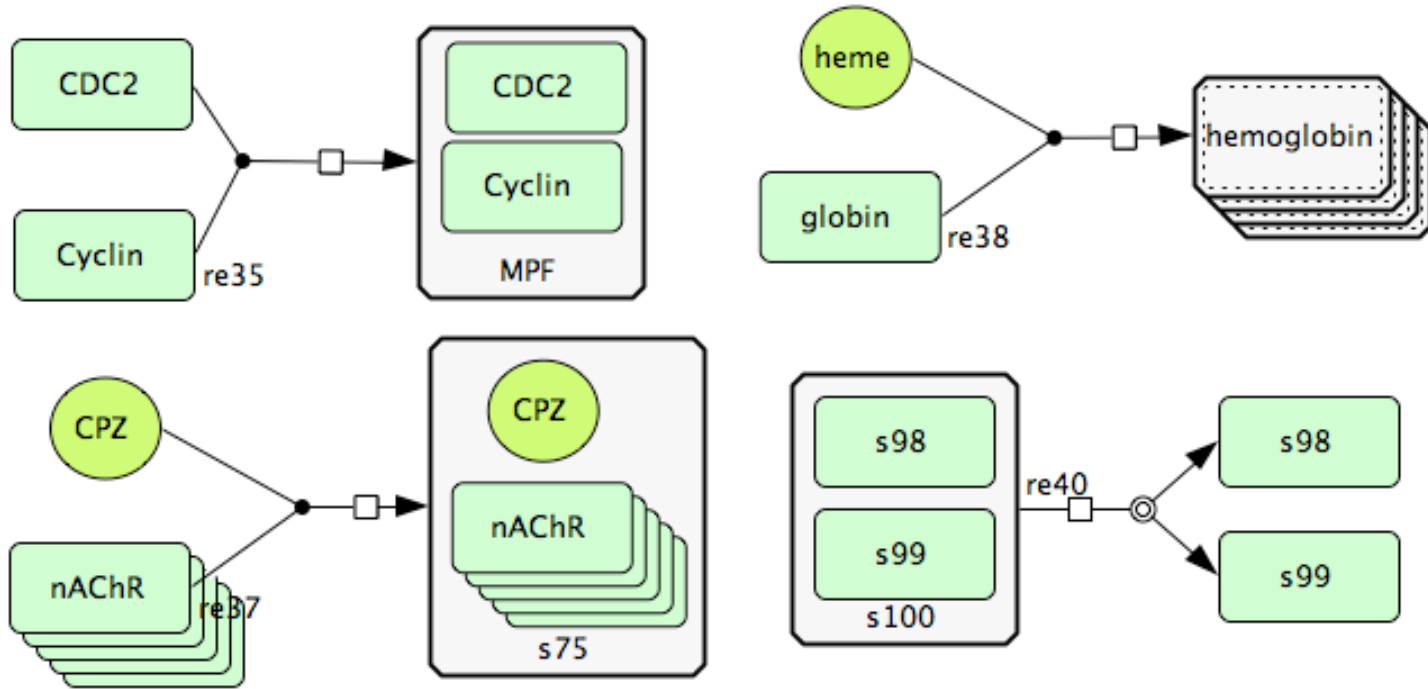
Graphical Notation

2.3.1 Transition

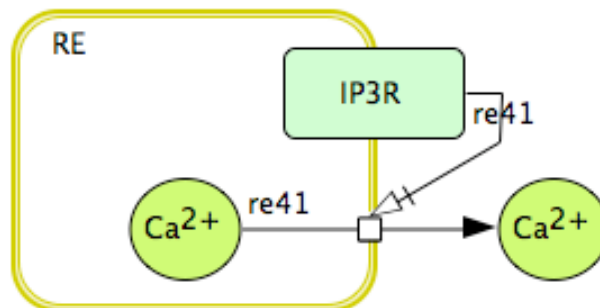


Graphical Notation

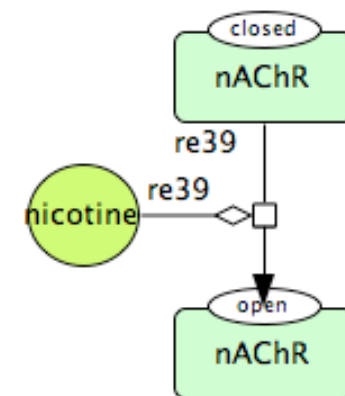
2.3.4 Association



2.4.7 Trigger



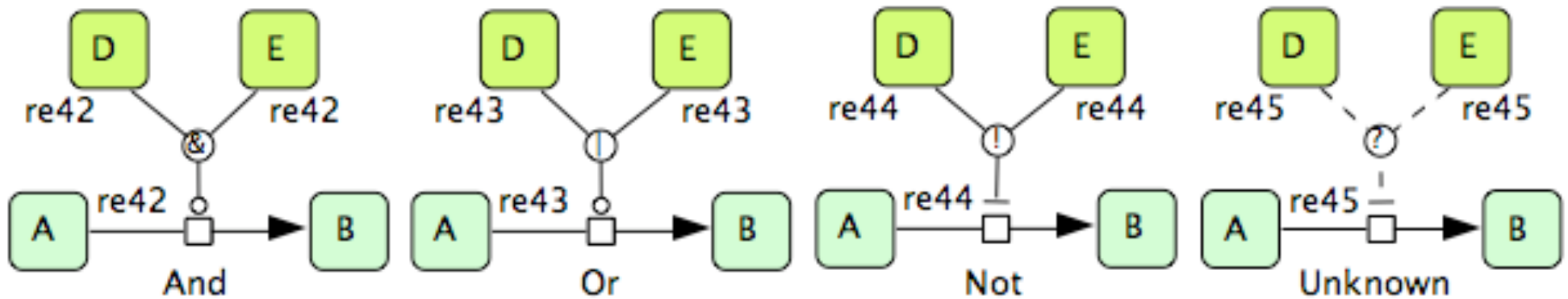
2.4.3 Modulation



Graphical Notation

● ‘&’ → “and”, ‘|’ → “or”, etc.

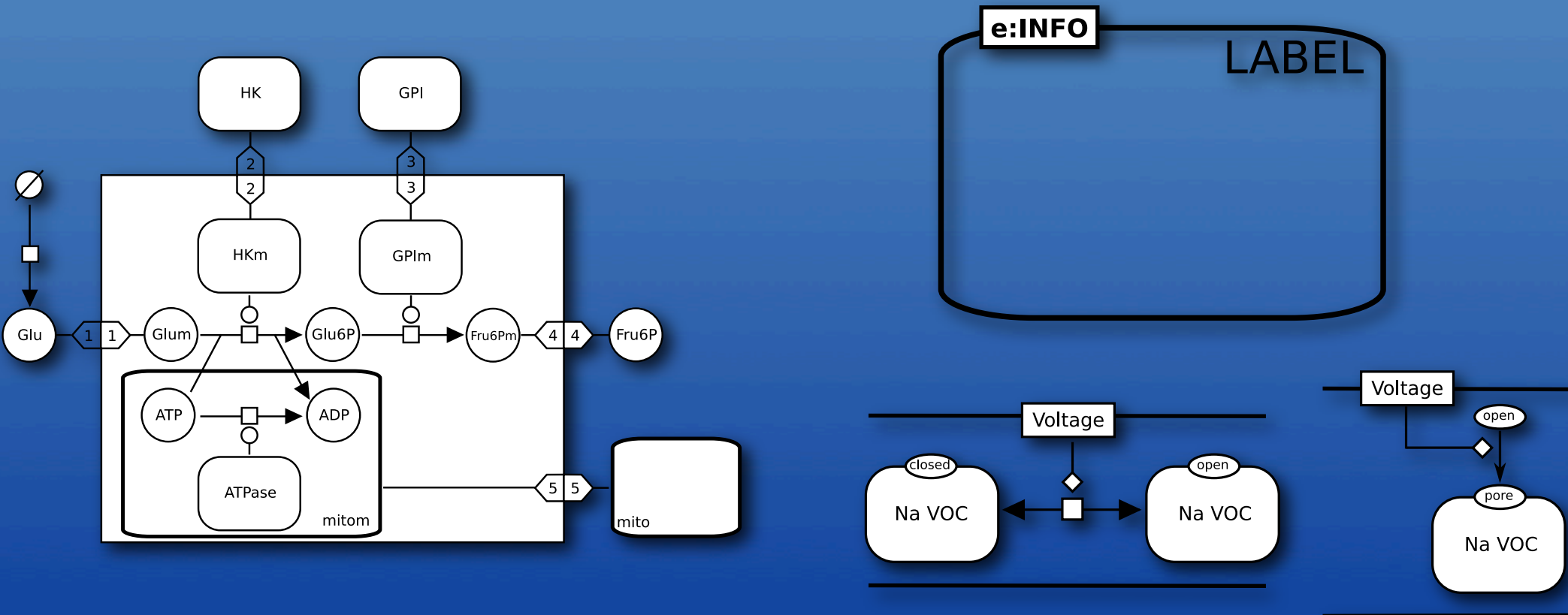
2.5 Logical Operators



● Todo:

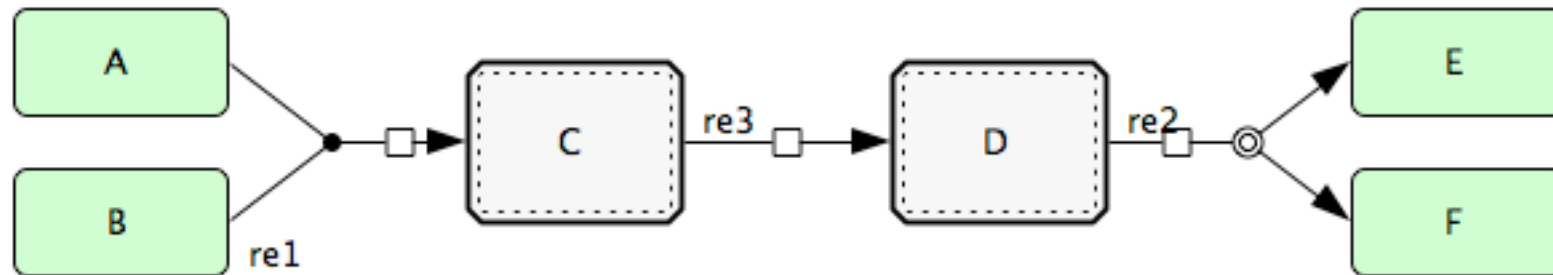
● Module

● Compartment (not fully supported)



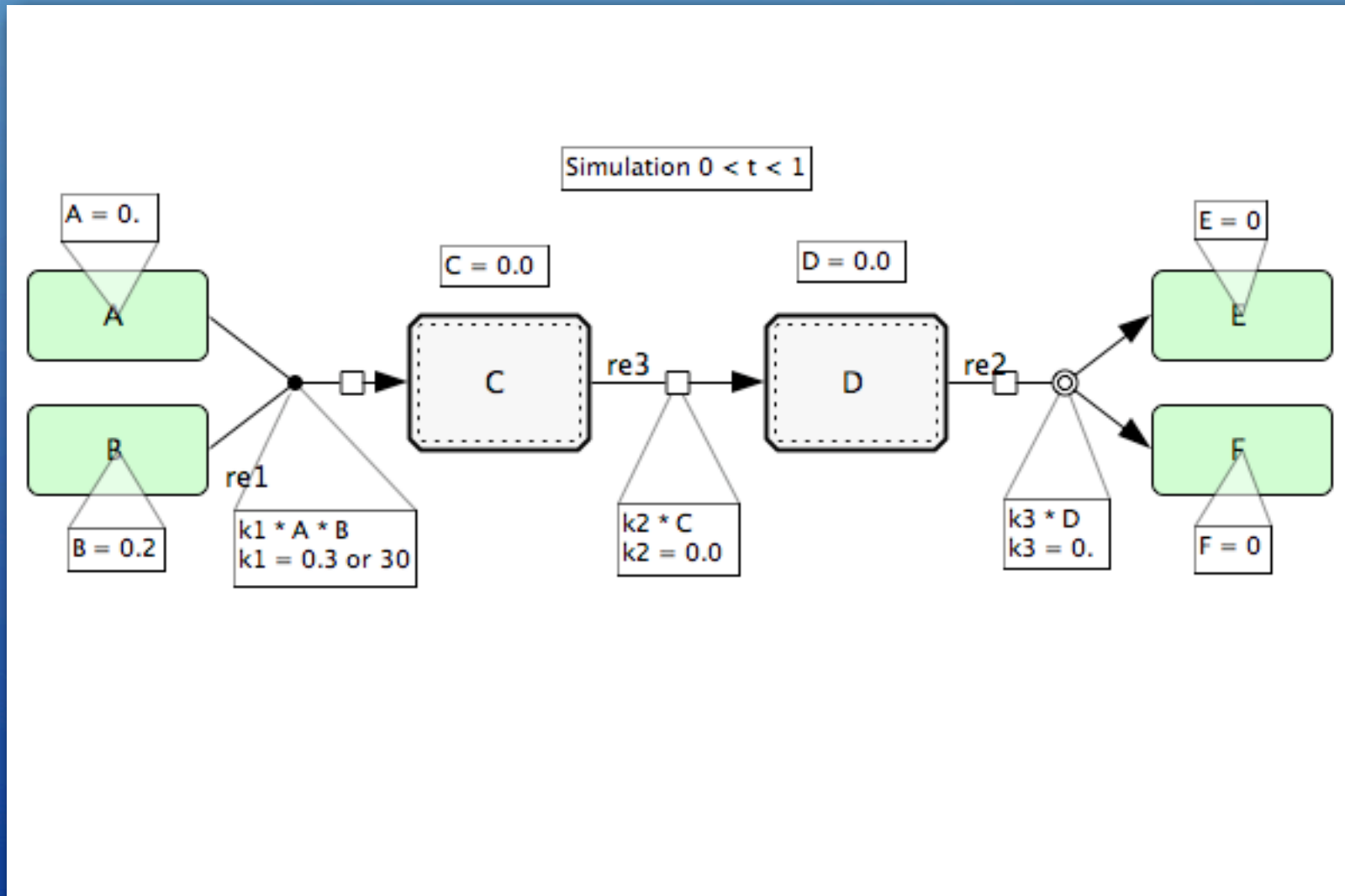
Layers

- Can add graphical / text object to your model

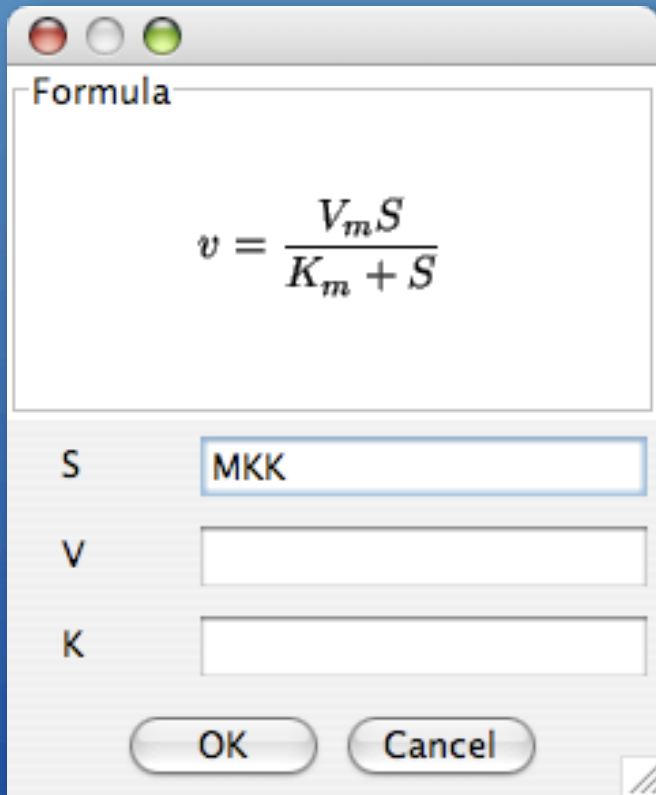


Layers

- Can add graphical / text object to your model



Enhanced Kinetic Law Editor



KineticLaw

math: $\frac{k3 * MKKK_P * MKK}{KK3 + MKK}$

timeUnits:

substanceUnits:

SelectedReaction

Predefined Functions

$v = \frac{V_m S}{K_m + S}$

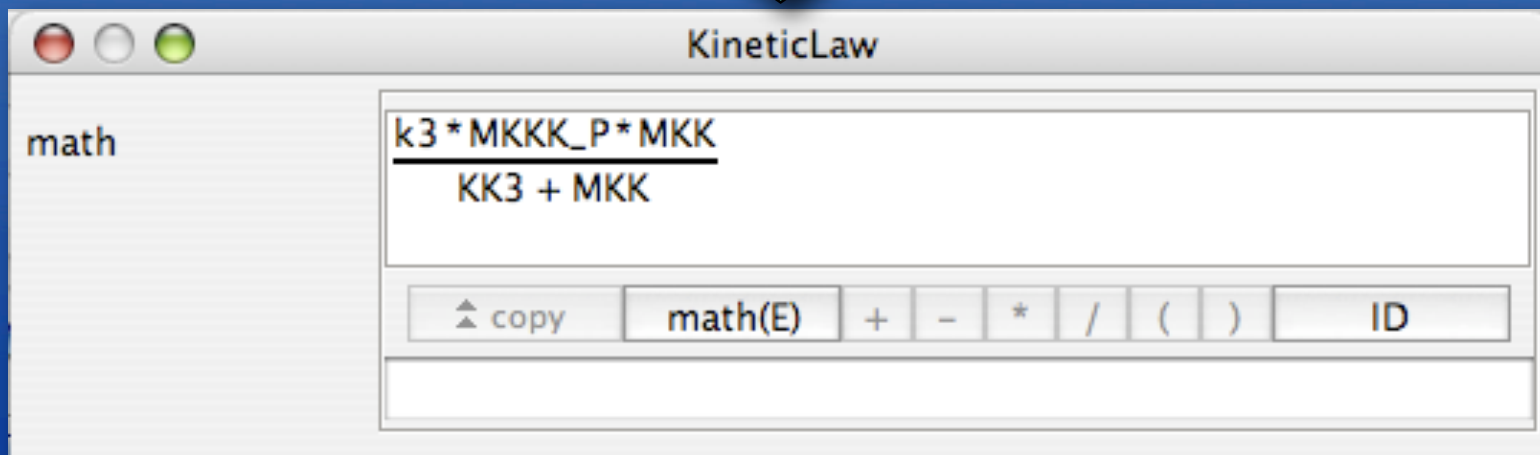
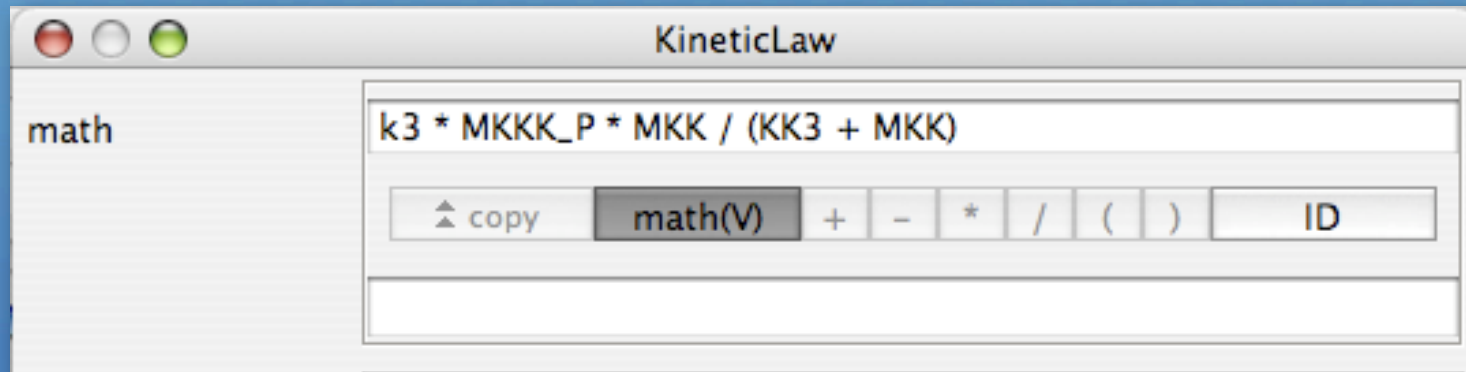
Species Parameters Rules

class	positionT...	id	name	compart...	quantity t...	initial...	substa...	sp
PROTEIN	inside	MKK	MKK	uVol	Amount	280.0		
PROTEIN	inside	MK... MKKK	MK... MKKK	uVol	Amount	90.0		
PROTEIN	inside	MAPK	MAPK	uVol	Amount	280.0		
PROTEIN	inside	MK... MKKK	MK... MKKK	uVol	Amount	10.0		
PROTEIN	inside	MK... MKK	MK... MKK	uVol	Amount	10.0		
PROTEIN	inside	MK... MKK	MK... MKK	uVol	Amount	10.0		

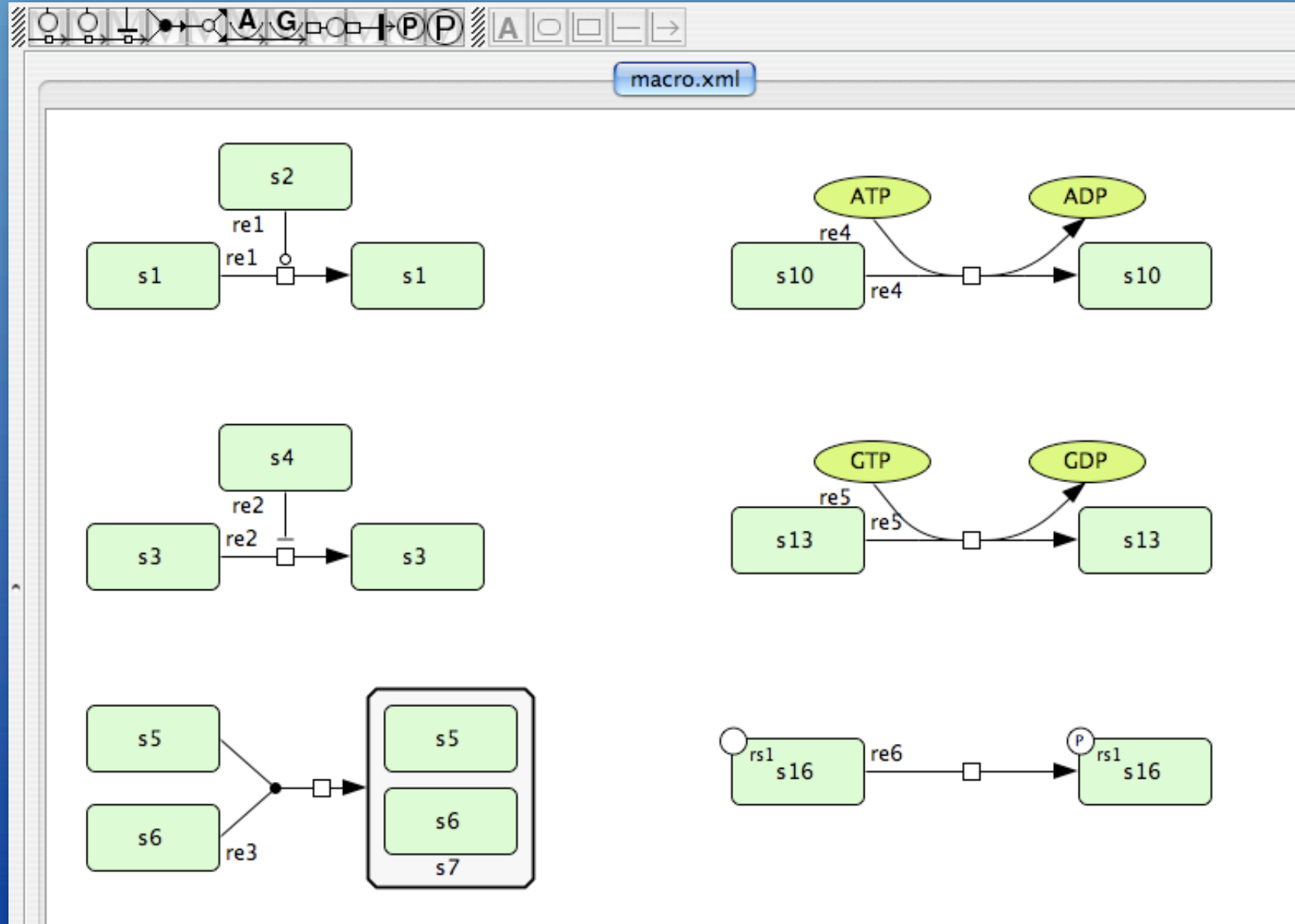
Update Close

GUI improvement

Enhanced Kinetic Law Editor



Macros



Plugin development

- Develop your plugin on Eclipse
- Call plugin from [Plugin] menu on CellDesigner

```

private JLabel jLabelY = null;
private JTextField textName = null;
private JTextField textId = null;
private JTextField textX = null;
private JTextField textY = null;
private JPanel jPanel = null;
private JButton jButtonGET = null;
private JButton jButtonADD = null;

public static SamplePlugin plug;

/**
 * This is the default constructor
 */
public SamplePluginDialog(SamplePlugin _plugin) {
    plug = _plugin;
    initialize();
}

public SamplePluginDialog(Frame arg0) throws HeadlessException {
    initialize();
}

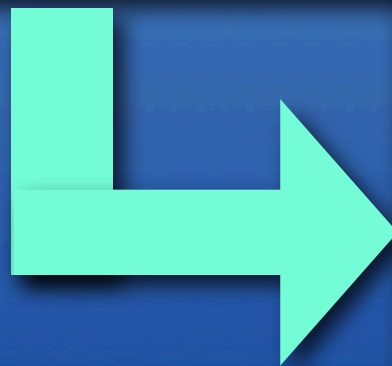
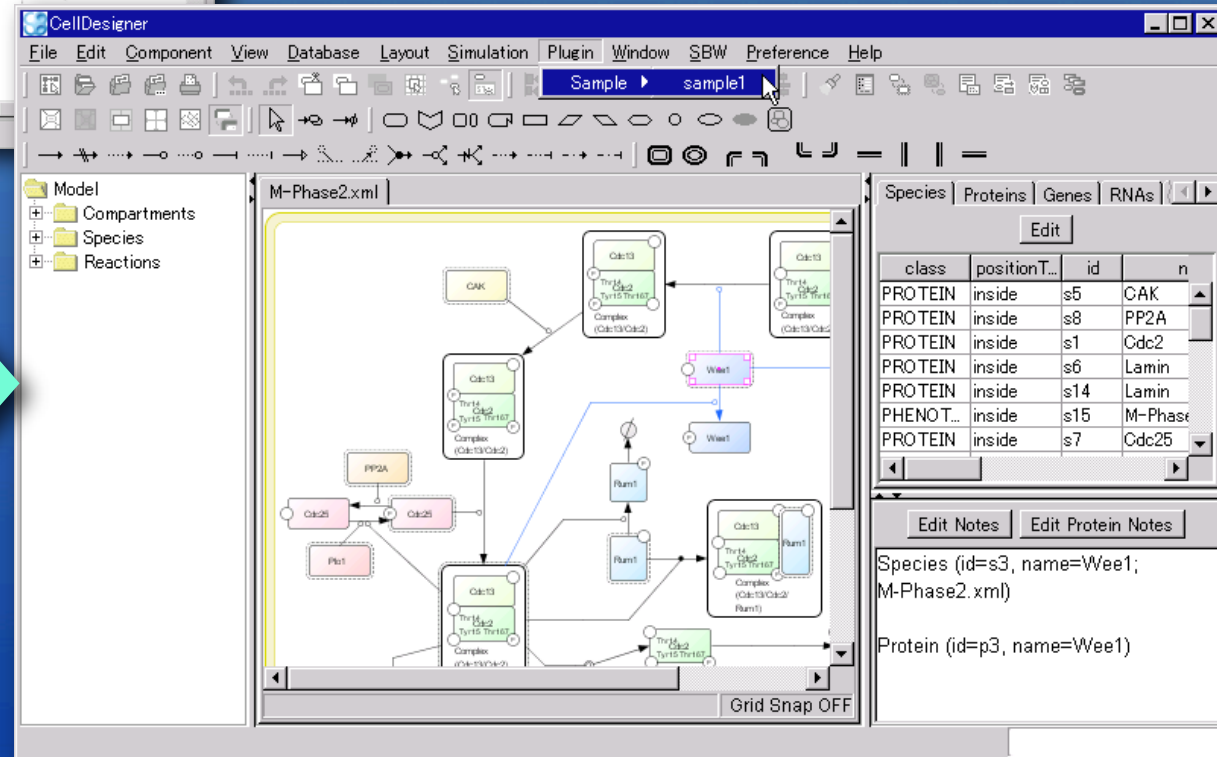
public SamplePluginDialog(Frame arg0, boolean arg1)
    throws HeadlessException {
    initialize();
}
    
```

```

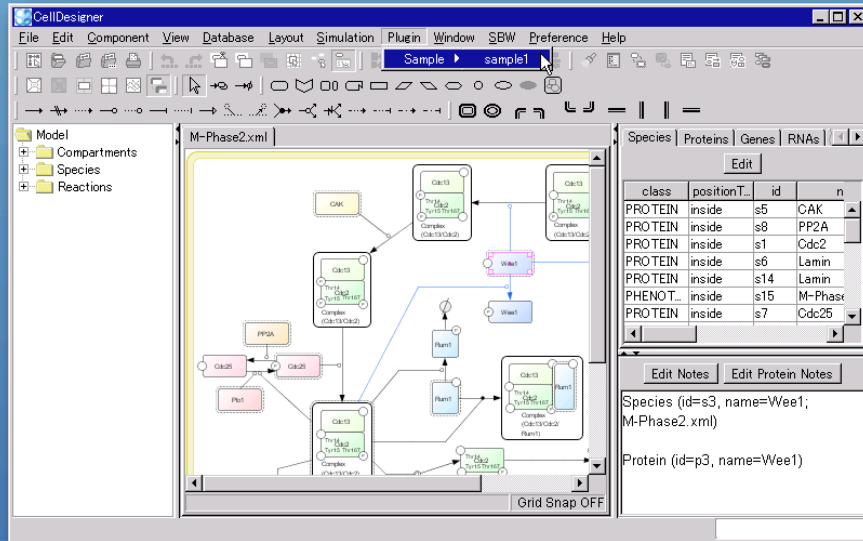
public class SamplePlugin extends CellDesignerPlugin {

    PluginMenuItem item;

    /**
     *
     */
    }
    
```



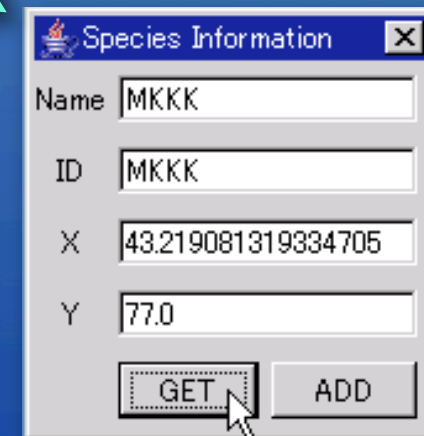
Plugin



CellDesigner

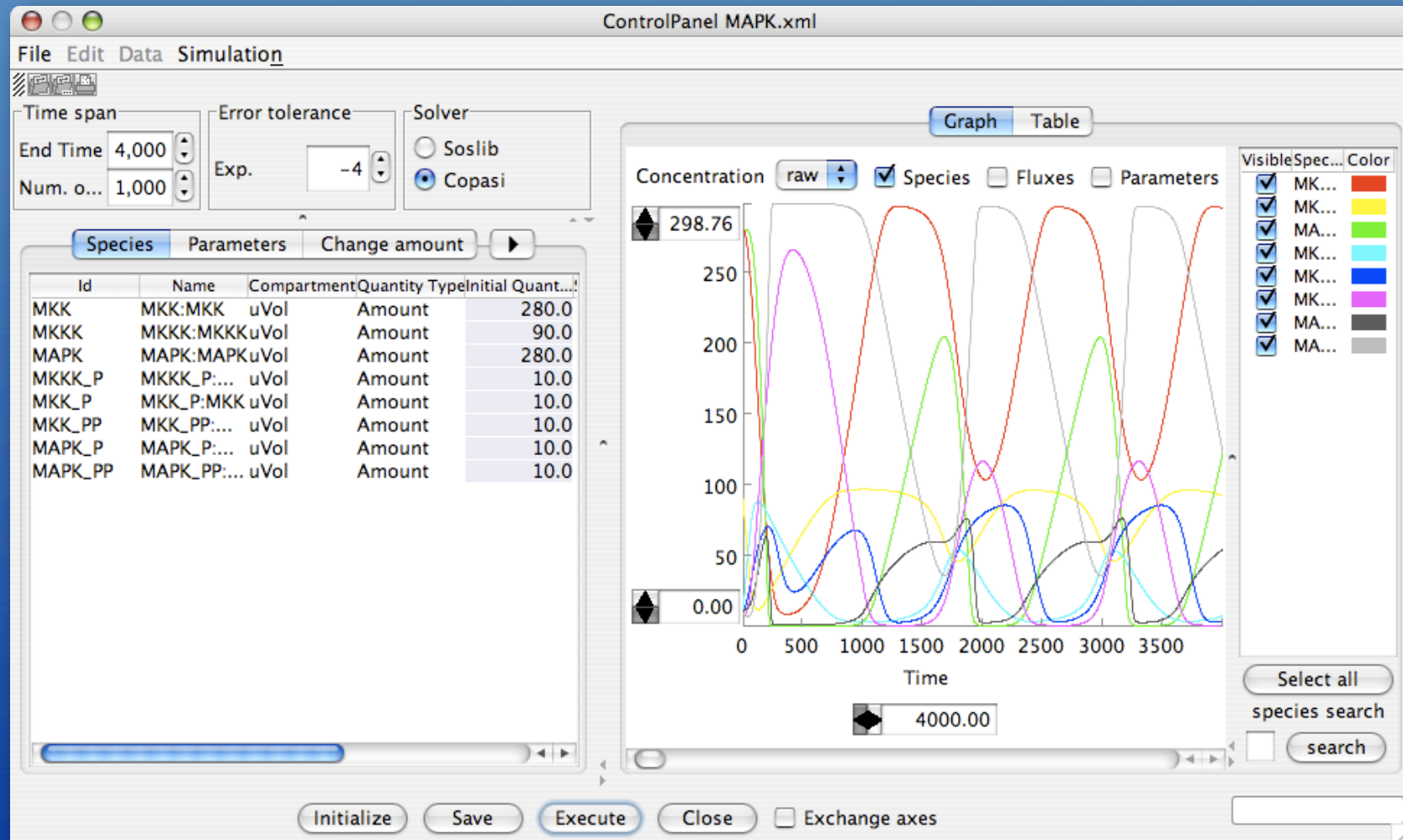
- Get object (species, reaction, etc.) information

- Add / modify object (species, reaction, etc.)



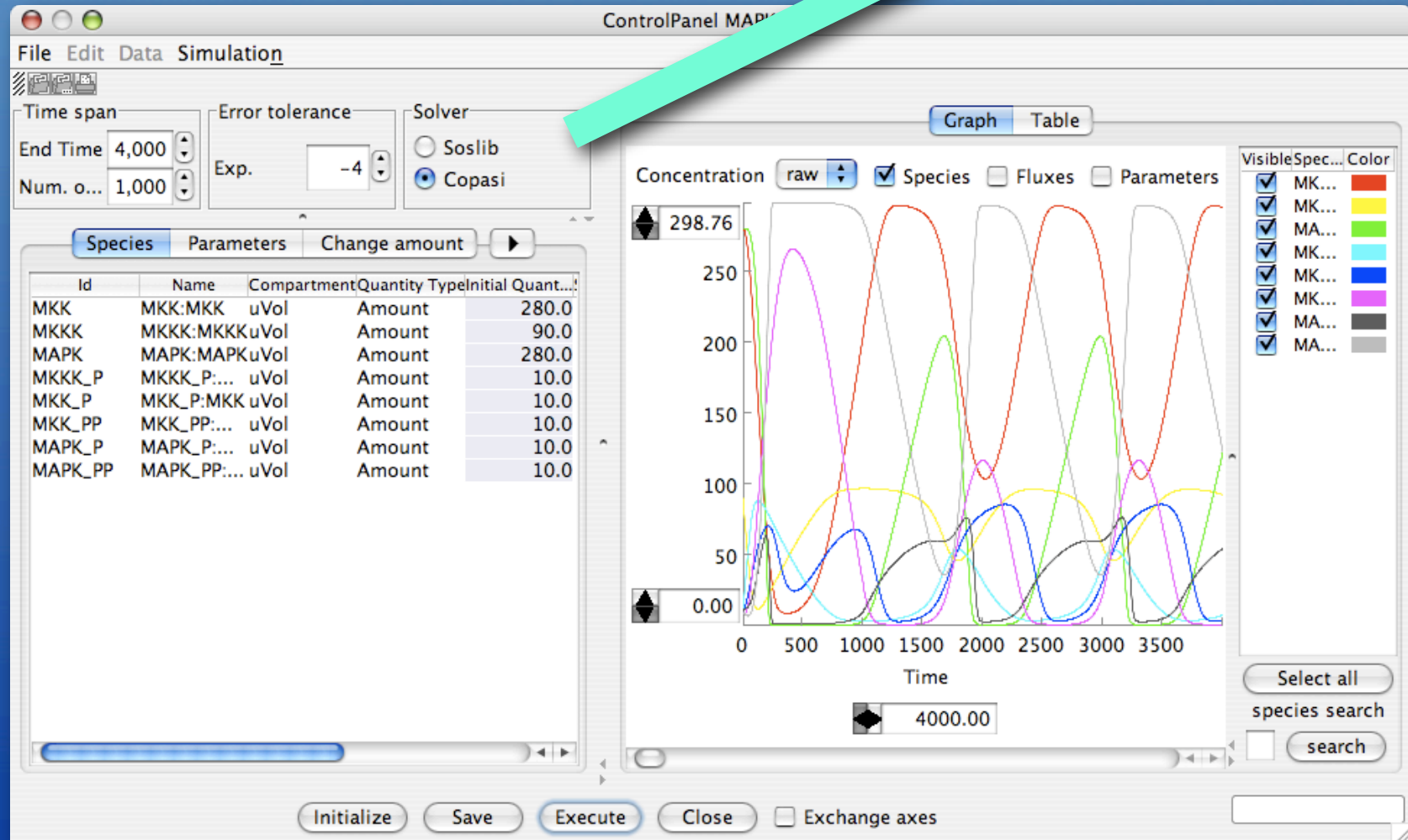
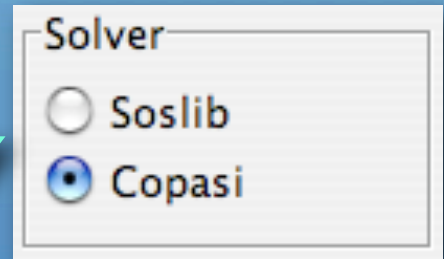
Plugin

- Can call COPASI directly from CellDesigner



COPASI - CellDesigner

Can call COPASI directly from CellDesigner



Future plan

- Support SBGN Level-1
- Support SBML L2v3 (libSBML 3.x)
- Integrate with COPASI
- Integrate with SABIO-RK
- Include current CVS version of SOSlib

Acknowledgment

SBML

- * SBML community

SBGN

- * SBGN community

CellDesigner

- * SBI

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Akiya Jouraku

- * MKI

Norihiro Kikuchi

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- * Christoph Flamm

SBW (Univ. of Washington)

- * Frank Bergmann
- * Herbert Sauro

COPASI (Univ. of Heidelberg)

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- * Sven Sahle
- * Ursula Kummer

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- * Saqib Mir
- * Isabel Rojas