Our Team

10 members
Goal

synthetic biology around the world!

By iGzME

Big Project!
Amateurs!

Designed for Modeling and Simulating tool

Designed for Amateurs!
Tools

Other modeling software

- TinkerCell
- SynBioSS
- CellDesigner

What's the Differences?
An oscillator

Example
Example

TinkerCell

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**Network 1**

- Molecules: m1, P1, P2, P3
- Parts: J1, J2, J3, J4, J5, J6, J7, J8, J9, J10, J11, J12, J13, J14, J15, J16, J17, J18, J19, J20, J21, J22, J23, J24, J25, J26, J27, J28, J29, J30, J31, J32, J33, J34, J35, J36
- Compartments: e1, e2, e3, e4, e5, e6, e7
- Modules: RNA, Protein, Phosphate, Transcription Factor, Receptor, Reporter, mRNA, Ribozyme

**Tools Window**

- Tools: Sequence, Generate kinetics, Analysis, Network structure, Database search, Steady state, Parameter scan, Optimize, Simulate

**Console Window**

```python
>>> Python initializing (init.py) ... DO NOT EXIT AT THIS TIME
Python modules loaded: Numpy and Scipy
PySCeS and/or NetworkX were not found
```
Example

The Problem

Modelers have to know all details of the network
We Think…

Design

Auto Modeling…

Network!
Automatic Modeling
How do we achieve this?
Key Point:

Our New Database
<table>
<thead>
<tr>
<th>RxnID</th>
<th>Reaction</th>
<th>Kinetic Data</th>
<th>Add</th>
<th>Edit</th>
<th>More Info</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1 RNAp + 2 tetO + 1 LacO + 1 P_AND → 1 RNAp:P_AND</td>
<td>100000000 L^3mol^3s^-1</td>
<td></td>
<td></td>
<td>Show</td>
</tr>
<tr>
<td>2</td>
<td>2 Lac1 → 1 Lac12</td>
<td>1000000000 L^1mol^1s^-1</td>
<td></td>
<td></td>
<td>Show</td>
</tr>
<tr>
<td>3</td>
<td>1 Lac12 → 2 Lac1</td>
<td>10 s^-1</td>
<td></td>
<td></td>
<td>Show</td>
</tr>
<tr>
<td>4</td>
<td>2 Lac12 → 1 Lac14</td>
<td>1000000000 L^1mol^1s^-1</td>
<td></td>
<td></td>
<td>Show</td>
</tr>
<tr>
<td>5</td>
<td>1 Lac14 → 2 Lac12</td>
<td>10 s^-1</td>
<td></td>
<td></td>
<td>Show</td>
</tr>
<tr>
<td>6</td>
<td>1 Lac14 + 1 LacO → 1 Lac14:LacO</td>
<td>2000000000 L^1mol^1s^-1</td>
<td></td>
<td></td>
<td>Show</td>
</tr>
<tr>
<td>7</td>
<td>1 Lac14:LacO → 1 Lac14 + 1 LacO</td>
<td>0.04 s^-1</td>
<td></td>
<td></td>
<td>Show</td>
</tr>
<tr>
<td>8</td>
<td>2 TetR → 1 TetR2</td>
<td>0.001 L^1mol^1s^-1</td>
<td></td>
<td></td>
<td>Show</td>
</tr>
<tr>
<td>9</td>
<td>1 TetR2 → 2 TetR</td>
<td>10 s^-1</td>
<td></td>
<td></td>
<td>Show</td>
</tr>
<tr>
<td>10</td>
<td>2 AraC → 1 AraC2</td>
<td>1000000000 L^1mol^1s^-1</td>
<td></td>
<td></td>
<td>Show</td>
</tr>
<tr>
<td>11</td>
<td>1 AraC2 → 2 AraC</td>
<td>10 s^-1</td>
<td></td>
<td></td>
<td>Show</td>
</tr>
<tr>
<td>12</td>
<td>1 AraC2 + 1 AraO → 1 AraC2:AraO</td>
<td>100000000 L^1mol^1s^-1</td>
<td></td>
<td></td>
<td>Show</td>
</tr>
<tr>
<td>13</td>
<td>1 AraC2:AraO → 1 AraC2 + 1 AraO</td>
<td>0.004 s^-1</td>
<td></td>
<td></td>
<td>Show</td>
</tr>
<tr>
<td>14</td>
<td>1 TetR2 + 1 tetO → 1 TetR2:tetO</td>
<td>1000000000 L^1mol^1s^-1</td>
<td></td>
<td></td>
<td>Show</td>
</tr>
<tr>
<td>17</td>
<td>1 TetR2:tetO → 1 TetR2 + 1 tetO</td>
<td>0.001 s^-1</td>
<td></td>
<td></td>
<td>Show</td>
</tr>
<tr>
<td>18</td>
<td>1 RNAp + 1 LacP + 1 LacO → 1 RNAp:LacP</td>
<td>20000000 L^2mol^2s^-1</td>
<td></td>
<td></td>
<td>Show</td>
</tr>
<tr>
<td>19</td>
<td>1 RNAp + 1 TetP + 1 tetO → 1 RNAp:TetP</td>
<td>8600000 L^2mol^2s^-1</td>
<td></td>
<td></td>
<td>Show</td>
</tr>
<tr>
<td>21</td>
<td>1 RNAp:TetP → 1 RNAp:TetP^*</td>
<td>0.13 s^-1</td>
<td></td>
<td></td>
<td>Show</td>
</tr>
<tr>
<td>22</td>
<td>1 RNAp:TetP + 1 RNAp + 1 TetP + 1 tetO</td>
<td>0.1 s^-1</td>
<td></td>
<td></td>
<td>Show</td>
</tr>
<tr>
<td>23</td>
<td>1 AraP + 1 RNAp + 2 AraO → 1 RNAp:AraP</td>
<td>2000000000 L^2mol^2s^-1</td>
<td></td>
<td></td>
<td>Show</td>
</tr>
<tr>
<td>24</td>
<td>1 RNAp:AraP → 1 RNAp:AraP^*</td>
<td>0.167 s^-1</td>
<td></td>
<td></td>
<td>Show</td>
</tr>
</tbody>
</table>
Template Reaction

TetR2 + p(tetR) R0040 = TetR2
Example

$\text{TetR2} + \text{pTetR} \rightarrow \text{pTetR:TetR2}$
chain
Chain

chain

Part Part Part
Just as BioBricks
DNA with pTetR
DNA with pTetR

Real BioBricks!
Chain

DNA with pTetR

pTetR → RBS → CDS → TE

Extend

IPTG → Compounds

E.coli → Compartments
Chain

DNA with pTetR

Basic Assumption:
Property preserves!
Chain

DNA with pTetR

Basic Assumption:
Property preserves!

Bring challenges to algorithm...
TetR dimer

Node

TetR

TetR
TetR dimer

Node

TetR

TetR

Node

binding site

links
Nodes can be bound again
The Reaction

Node

TetR2

Node

pTetR:TetR2

Node

pTetR

TetR

TetR

RBS  CDS  TE

RBS  CDS  TE
Template Substituent
Substituent

Template

Represents other parts

Similar in chemistry

\[
\text{ANY} \quad \text{pTetR} \quad \text{ANY}
\]

\[
\text{X: Cl, Br}
\]
Template

Substituent

ANY

Part
Part
Part

one chain
Rewrite it!

Template

Using any

pTetR
RBS
CDS
TE

ANY
pTetR
ANY
Rewrite it!

Using any

Template Species!
Match!

Template Species!
Template

One for all!

Template Reaction!

TetR2

Node

pTetR:TetR2

Node

pTetR
Template Reaction

DB

Structural Mechanism
reuse!
MoDeL Standardization

Machine-readable
XML fashion

MoDeL

Standard biological parts automatic Modeling Database Language

RFC 55
XML Schema
**Biological processes:**

- Reactions with forward and reverse parts
- Multi-compartment reaction
- Cell reproduction
- Dilution of species
- Plasmid replication and repression
- Description of environmental conditions
MoDeL

Organization

- **Compartment**: holder of substance with certain volume
- **Part**: basic elements for other components of MoDeL
- **System**: other components of MoDeL
- **Species**: other components of MoDeL
- **Reaction**: other components of MoDeL
MoDeL Connection

- Compartiment
- Part
- Species
- Reaction
- System
Algorithm

Challenge

How to recognize a specific structure in a BIG species
Both Match!
Algorithms of:

- Chain Sorting and Weighting
- Matching of structural pattern
- Generation of products based on reaction templates

Learn more on wiki
Workflow

Start!

Read Input

Read next species

Is there any matching template species in DB?

Y

N

Read next species

Is there any matching template species in DB?

Y

Search linked template reactions

Do the other reactions and modifiers exist?

N

Y

Are the reaction parameter conditions satisfied?

N

Y

Add products

Add the reaction

Reach the end of species list?

N

Y

End
Demo

pLux-LuxR repression system
Future

**Next version of MoDeL**
- Enhance MoDeL to support description of intra-molecular reactions.
- More powerful substituent.
- Enable description of transcription and translation reactions.

**New functions of iGaME**
- Various and elegant output for both professionals and amateurs.
- More friendly user interface with fun.
- Online and multiplayer cooperation.
- Database Development Kit.
- More entertainment, more excitement, more experience!
Summary

The Idea

Automatic Modeling

The Standard

MoDeL

The Software

iGaME
Acknowledgments

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➢ Zhaofeng Luo
➢ Hao Jiang

Open source codes we use in our software
Questions are Welcome!