

BiVeS & BudHat

Version Control for Computational Models

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Motivation

Detecting Differences

Visualizing Differences

Conclusions

Done



Motivation

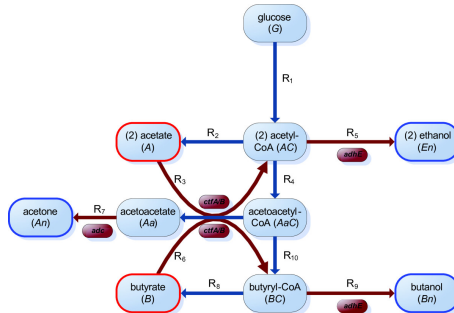
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metabolic and gene regulation network model in *C. acetobutylicum*



Haus *et. al.* 2011



Papoutsakis



Equations and calculations for fermentations of butyric acid bacteria
1984 in *Biotechnology and bioengineering*

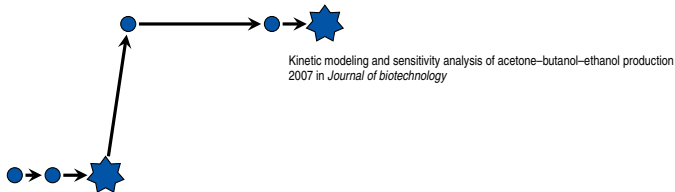


time

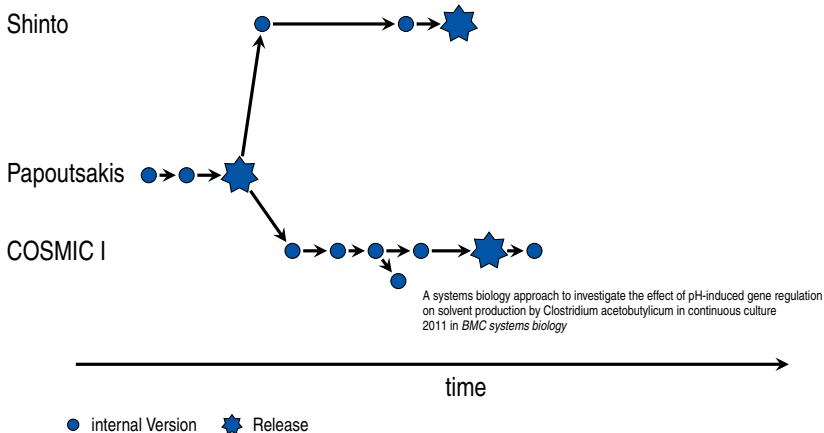
● internal Version ★ Release

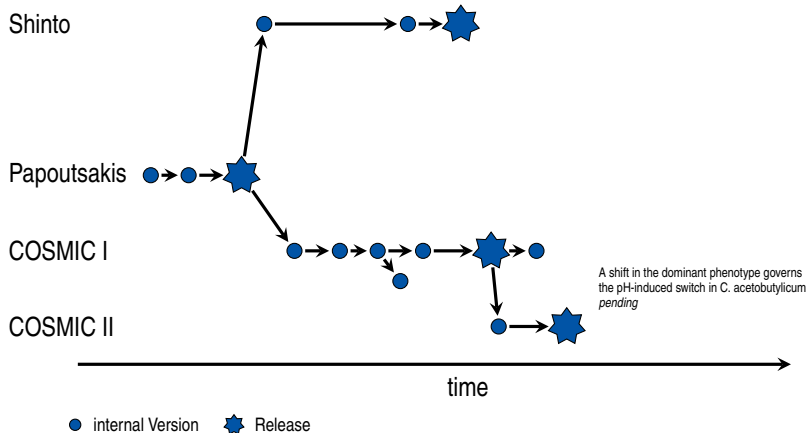
Shinto

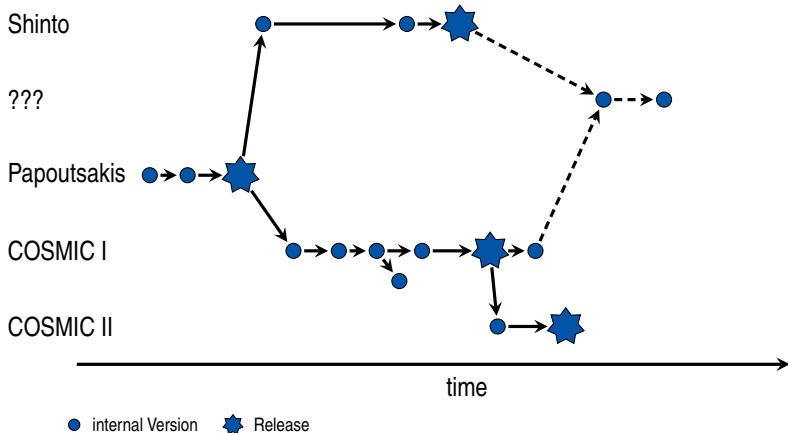
Papoutsakis

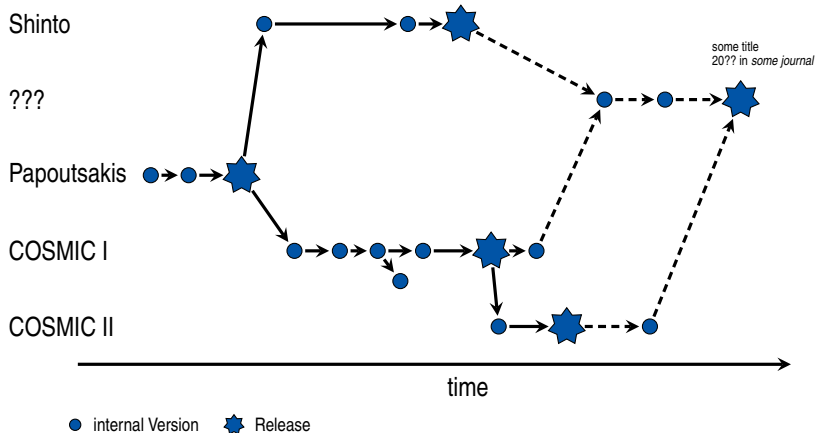


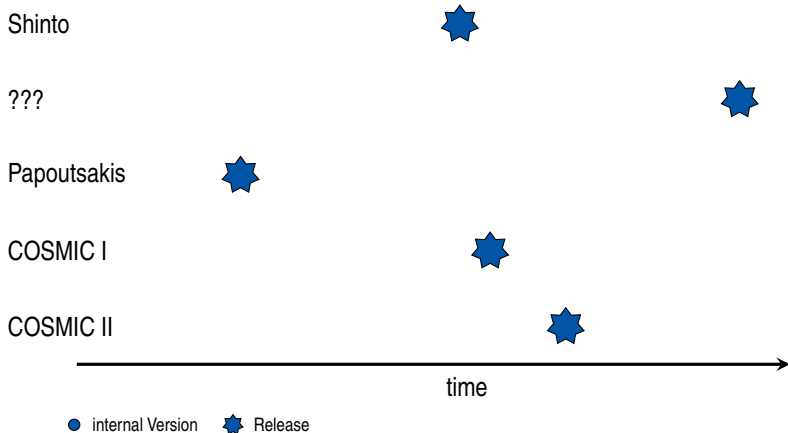
● internal Version ★ Release

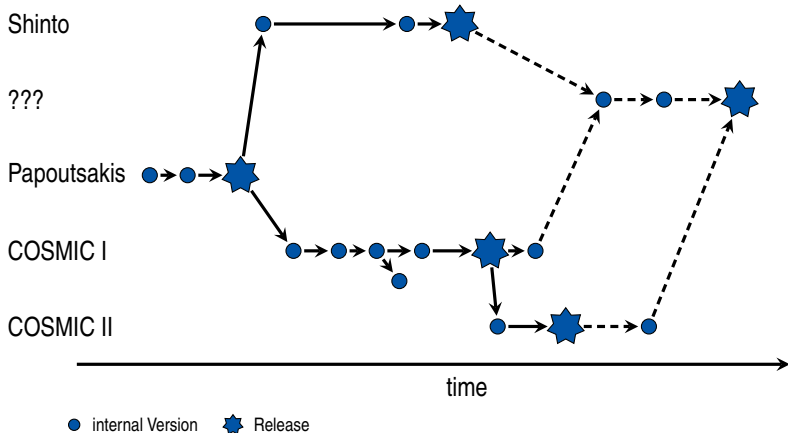














- Unambiguously identifiable models
- Robust difference detection
- Interpretation and justification of identified changes



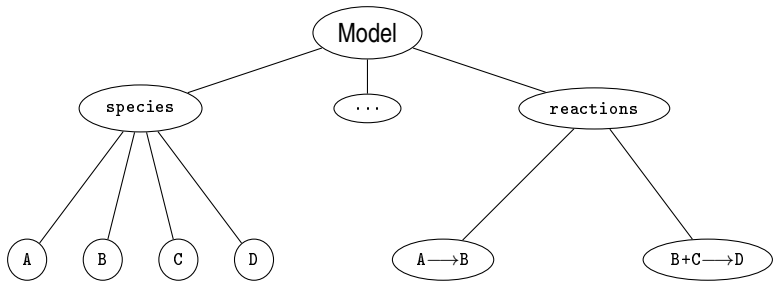
Motivation

Detecting Differences

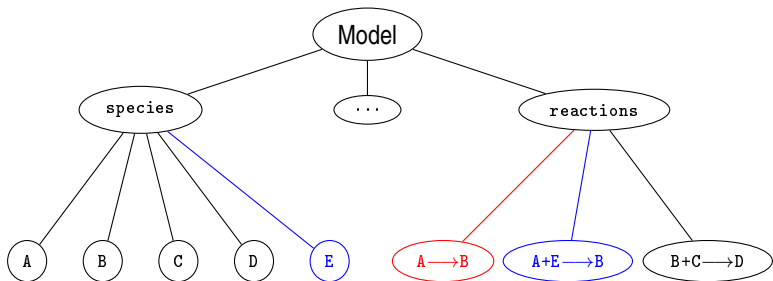
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Model is encoded in XML



We are interested in changes of the entities!

Generating a diff using Unix' diff-tool is very useful for various things:

- text (notes, latex etc)
- source code
- ...

```
22  def salute
23  puts "Hello?"
24  end
```

 VS

```
22  def salute
23  puts "Hello!"
24  end
```

```
23c23
< puts "Hello?"
- - -
> puts "Hello!"
```

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- text (notes, latex etc)
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```
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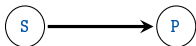
```
22  def salute
23    puts "Hello!"
24  end
```

```
23c23
< puts "Hello?"
- - -
> puts "Hello!"
```

⇒ content that is **line-based**

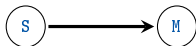
version A

```
<reaction id="StoP" fast="false">
  <listOfReactants>
    <speciesReference species="S"/>
  </listOfReactants>
  <listOfProducts >
    <speciesReference species="P"/>
  </listOfProducts>
</reaction>
```



version B

```
<reaction fast="false" id="StoP">
  <listOfReactants>
    <speciesReference species="S"/>
  </listOfReactants>
  <listOfProducts>
    <speciesReference species="M"/>
  </listOfProducts>
</reaction>
```



What does a resulting diff of these models reveal?

```
usr@srv ~ $ diff A B
1,7c1,7
< <reaction id="StoP" fast="false">
<   <listOfReactants>
<     <speciesReference species="S"/>
<   </listOfReactants>
<   <listOfProducts >
<     <speciesReference species="P"/>
<   </listOfProducts>
```

A

```
---
> <reaction fast="false" id="StoP">
>   <listOfReactants>
>     <speciesReference species="S"/>
>   </listOfReactants>
>   <listOfProducts>
> <speciesReference species="M"/>
>   </listOfProducts>
```

B

⇒ interesting parts are covered up in lots of irrelevant changes



How to identify changes in XML-encoded computational models?

How to interpret detected changes?

Bives = **B**iochemical Model **V**ersioning **S**ystem

Library to identify and classify changes between SBML-encoded models

- Adaptation of XyDiff (in collaboration with Robert Hälke)
- Input: 2 SBML models
- Output: Diff in XML format containing Diff operations:
 - Deletes
 - Inserts
 - Updates
 - Moves



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Budhat: Prototype for Version Control

- Display of the generated Diff
- Visualization of the model (in collaboration with Steffen Hadlak)

Project: BudHat

Welcome root! [logout](#)

available models

```

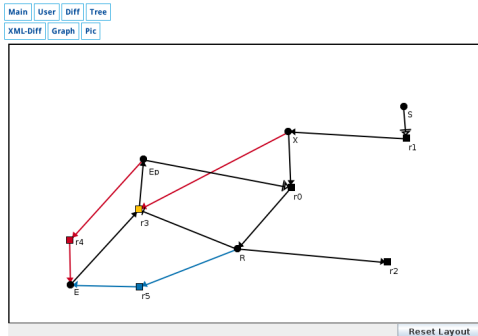
Novak1997_Ce11Cycle
2812-18-85 (L2V3)
test
2000-09-09 (L2V4)
2000-09-09 (L2V4)
oif
jaczesynth (L2V4)
ptinst (L2V4)
sigbrlysis (L2V4)
tracrhnb (L2V4)
  
```

selected models

```

test - 2222-22-22 (L2V4)
test - 2222-22-23 (L2V4)
  
```

compare





DEMO of BudHat using models from

Proteolysis of beta-galactosidase following SigmaB activation in *Bacillus subtilis*
Liebal *et. al.* 2012

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- Version control is beneficial
- We do not want to establish yet another platform for users

- Can SysMO/SEEK be improved by our tools?



That's it! Stay tuned ;-)

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<http://budhat.sems.uni-rostock.de>

Questions? Suggestions? Recommendations? Drop me an email:

martin.scharm@uni-rostock.de

