BiVeS & BudHat
Version Control for Computational Models

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Motivation

Detecting Differences

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

Haus *et. al.* 2011
Version Control for Models

Motivation

Papoutsakis

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

![Diagram showing time, internal version, and release]

- Internal Version
- Release
Motivation

Shinto

Papoutsakis

Kinetic modeling and sensitivity analysis of acetone–butanol–ethanol production 2007 in Journal of biotechnology
A systems biology approach to investigate the effect of pH-induced gene regulation on solvent production by Clostridium acetobutylicum in continuous culture 2011 in *BMC systems biology*
A shift in the dominant phenotype governs the pH-induced switch in C. acetobutylicum pending.
Version Control for Models

Motivation

Shinto

???

Papoutsakis

COSMIC I

COSMIC II

some title
20?? in some journal

time

internal Version Release
Version Control for Models

Motivation

- Shinto
- ???
- Papoutsakis
- COSMIC I
- COSMIC II

(time)

- internal Version
- Release
Version Control for Models

Requirements

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

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Done
let's take a short look at our models

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!"`
Generating a diff using Unix’ diff-tool is very useful for various things:

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

⇒ content that is **line-based**
What does a resulting diff of these models reveal?
Diff for XML

Appropriate for SBML versioning?

→ interesting parts are covered up in lots of irrelevant changes

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

A

B

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

Difference detection between models

How to identify changes in XML-encoded computational models?
How to interprete detected changes?
**Bives** = **Biochemical Model Versioning System**
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)
DEMOf BudHat using models from
Proteolysis of beta-galactosidase following SigmaB activation in *Bacillus subtilis*
Liebal et. al. 2012

http://budhat.sems.uni-rostock.de
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Done
Conclusions

- 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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Questions? Suggestions? Recommendations? Drop me an email:
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