

BiVeS & BudHat

Difference Detection for Computational Models

MARTIN SCHARM

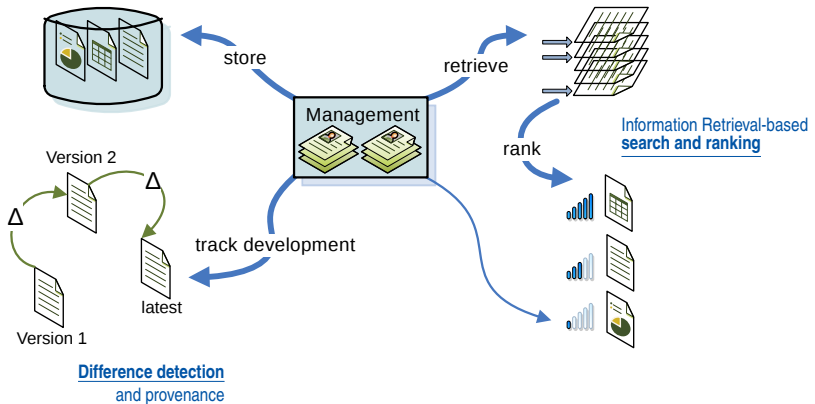
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University of Rostock

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



COMBINE 2013

Format-independent,
graph-based storage



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

Provenance represents the seven W's (Who, What, Where, Why, When, Which, (W)how).

– Goble 2002



Music
and Arts



Literature

REFERENCES

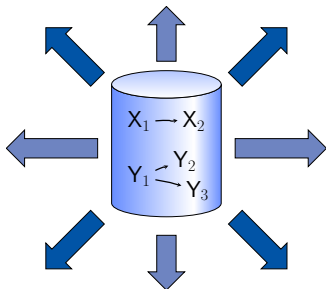
- Barclay, A., et al. (2009). COBOL: metadata standards, metadata tools and repository. *Provenance: From Theory to Practice*, 347–367. 10.1007/978-1-4419-1000-0_17.
- Chen, M., et al. (2010). Using provenance to track the provenance of information. *ACM SIGMOD Rec.*, 39, 497–504.
- Conrad, et al. (2011). High-throughput sequencing of cellular transcriptomes using microarrays. *Proc. Natl. Acad. Sci.*, 108, 107–112.
- Curran, A., et al. (2009). The COBOL standard 1.0 specification. <http://www.cobol.org/specifications/cobol-standard/cobol-standard-1.0>. Date last accessed: 2010-10-10.
- Curran, A., et al. (2009). An overview of COBOL 1.1, a biological model design language. *Genomics*, 94, 100–101.
- Faloutsos, K., et al. (2004). Computational challenges of system biology. *IEEE Comp.*, 37, 20–30.
- Goble, P. et al. (2010). Provenance: a language for describing data provenance. *Proc. ACM SIGMOD Rec.*, 39, 497–504.
- Henderson, J., et al. (2009). A formal model of provenance in system biology. *IEEE Transactions*, 58, 427–439.
- Henderson, J., et al. (2010). A formal model of provenance in system biology: a formal model of provenance and associated limitations. In: *Provenance: From Theory to Practice*, 347–367. 10.1007/978-1-4419-1000-0_17.
- Henderson, J., et al. (2010). A formal model of provenance in system biology: a formal model of provenance and associated limitations. In: *Provenance: From Theory to Practice*, 347–367. 10.1007/978-1-4419-1000-0_17.
- Henderson, J., et al. (2010). A formal model of provenance in system biology: a formal model of provenance and associated limitations. In: *Provenance: From Theory to Practice*, 347–367. 10.1007/978-1-4419-1000-0_17.
- Henderson, J., et al. (2010). A formal model of provenance in system biology: a formal model of provenance and associated limitations. In: *Provenance: From Theory to Practice*, 347–367. 10.1007/978-1-4419-1000-0_17.

```

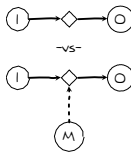
14  my $script = "
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```

Code



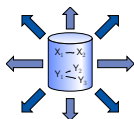
Availability & Identity



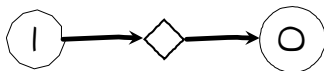
**Difference
Detection**



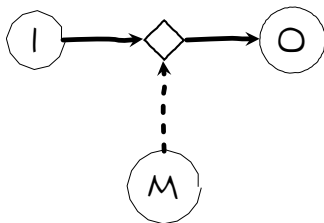
Interpretation



Availability
& Identity



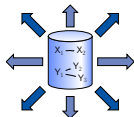
-vs-



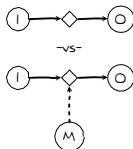
Difference Detection



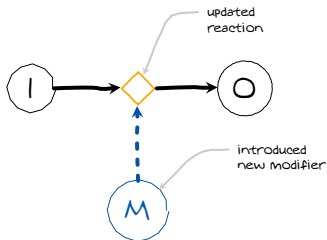
Interpretation



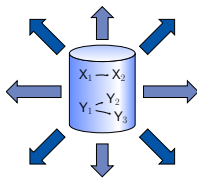
Availability
& Identity



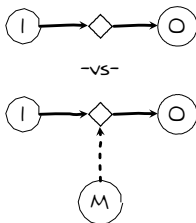
Difference
Detection



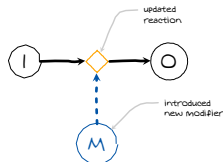
Interpretation



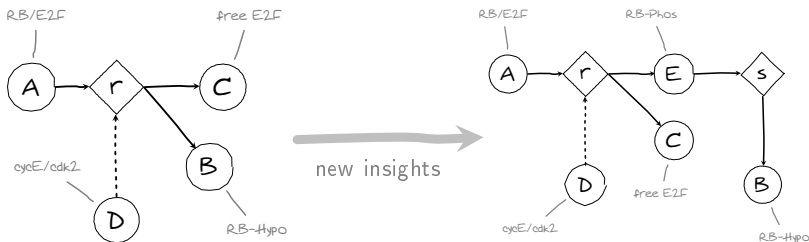
**Availability
& Identity**



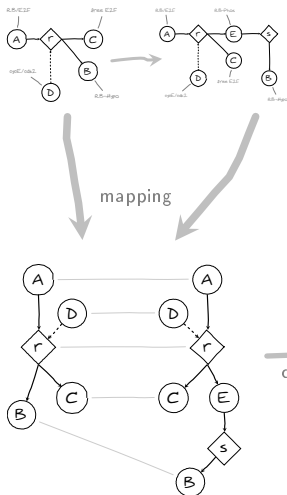
**Difference
Detection**





Interpretation



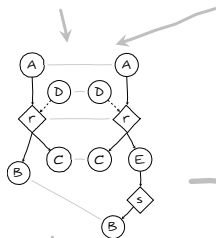
Waltemath *et al.*: Improving the reuse of computational models through version control. *Bioinformatics* (2013) 29(6): 742-728;




Biochemical Model Version Control System

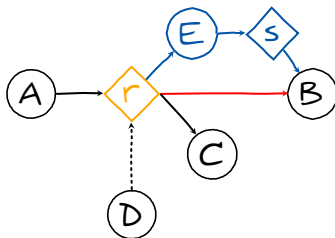
- compares models encoded in standardized formats (currently:  and )
- maps hierarchically structured content
- constructs a diff (in XML format)
- is able to interpret this diff

```
<XML>
Diff
├── moves
│   └── product of r: C
├── deletes
│   └── product of r: B
└── inserts
    ├── species: E
    ├── product of r: E
    └── reaction s
</XML>
```



```
<XML>
Diff
├── moves
│   └── product of r: C
├── deletes
│   └── product of r: B
├── inserts
│   ├── species: E
│   ├── product of r: E
│   └── reaction s
</XML>
```

- calls BiVeS to construct the diff
- displays the result in various formats
 - the XML diff
 - a reaction network highlighting the changes using 
 - a human readable report





BudHat in action!

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

jvm

network

cmd

```
import de.uni-rostock.sems.bives.api.SBMLDiff;

[...]
```

```
SBMLDiff differ = new SBMLDiff (sbmlFileA, sbmlFileB);
differ.mapTrees ();
String graph = differ.getCRNGraphML ();

[...]
```

jvm

network

cmd

```
curl -d '{
  "get":
  [
    "documentType",
    "xmlDiff"
  ],
  "files":
  {
    "versionA": "http://your.db/path/to/versionA.sbml",
    "versionB": "http://your.db/path/to/versionA.sbml"
  }
}' http://bives.server.tld
```

jvm

network

cmd

```
java -jar BiVeS.jar path/to/versionA path/to/versionB
```



```
git diff 88fealcddf b64477d742 model.file
```



- BiVeS = Difference detection for hierarchically structured content
- BudHat = Prototypic web interface to demonstrate how BiVeS can be used to communicate the differences

That's it! Stay tuned ;-)



@SemsProject

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

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

Questions? Suggestions? Recommendations? Drop me an email:

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