Universität Rostock Traditio et Innovatio

SYSTEMS BIOLOGY BIOINFORMATICS ROSTOCK

SEMS simulation experiment management system

The CellML models' walk through the repository

A retrospective study

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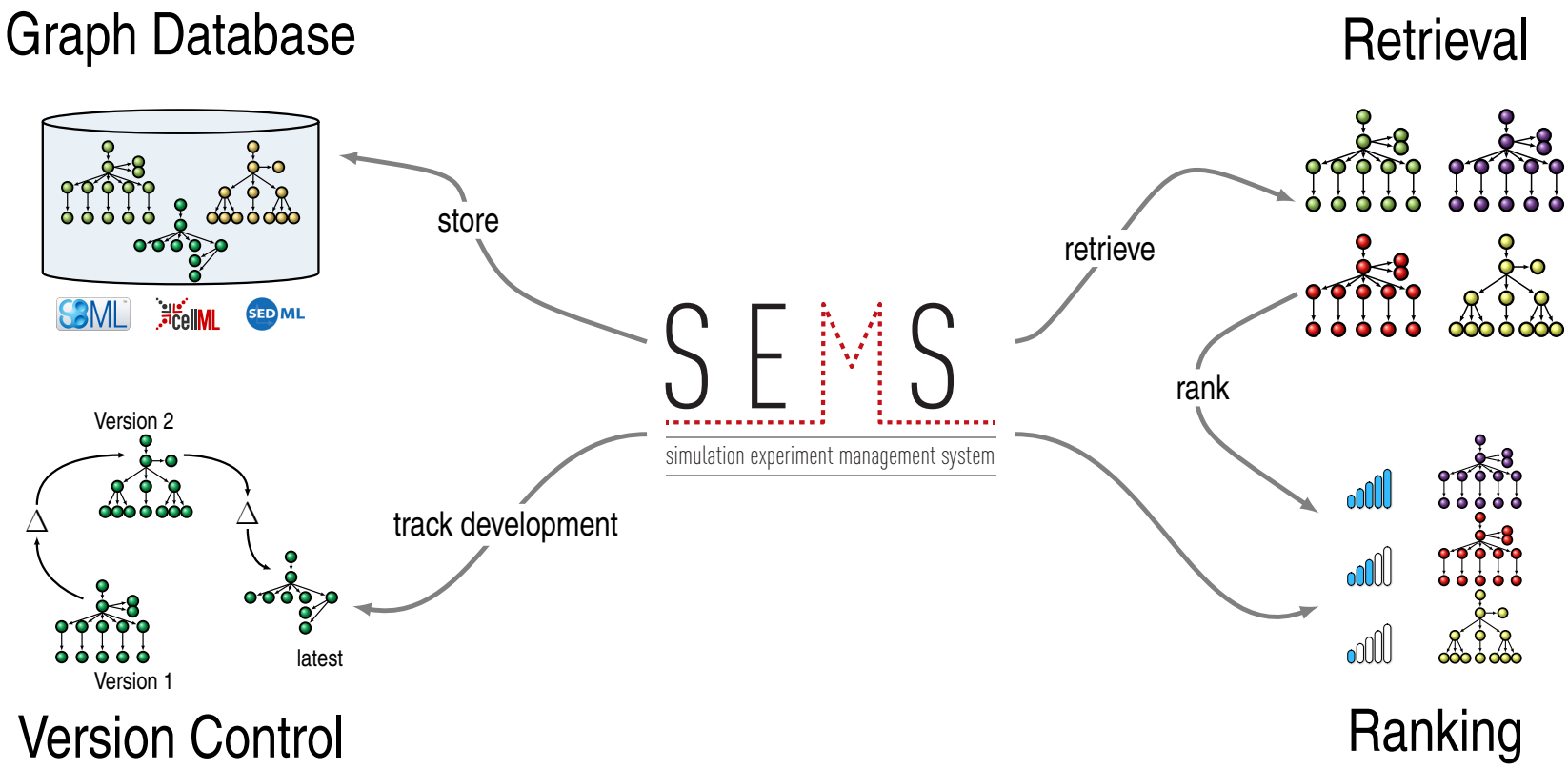
Department of Systems Biology & Bioinformatics, University of Rostock

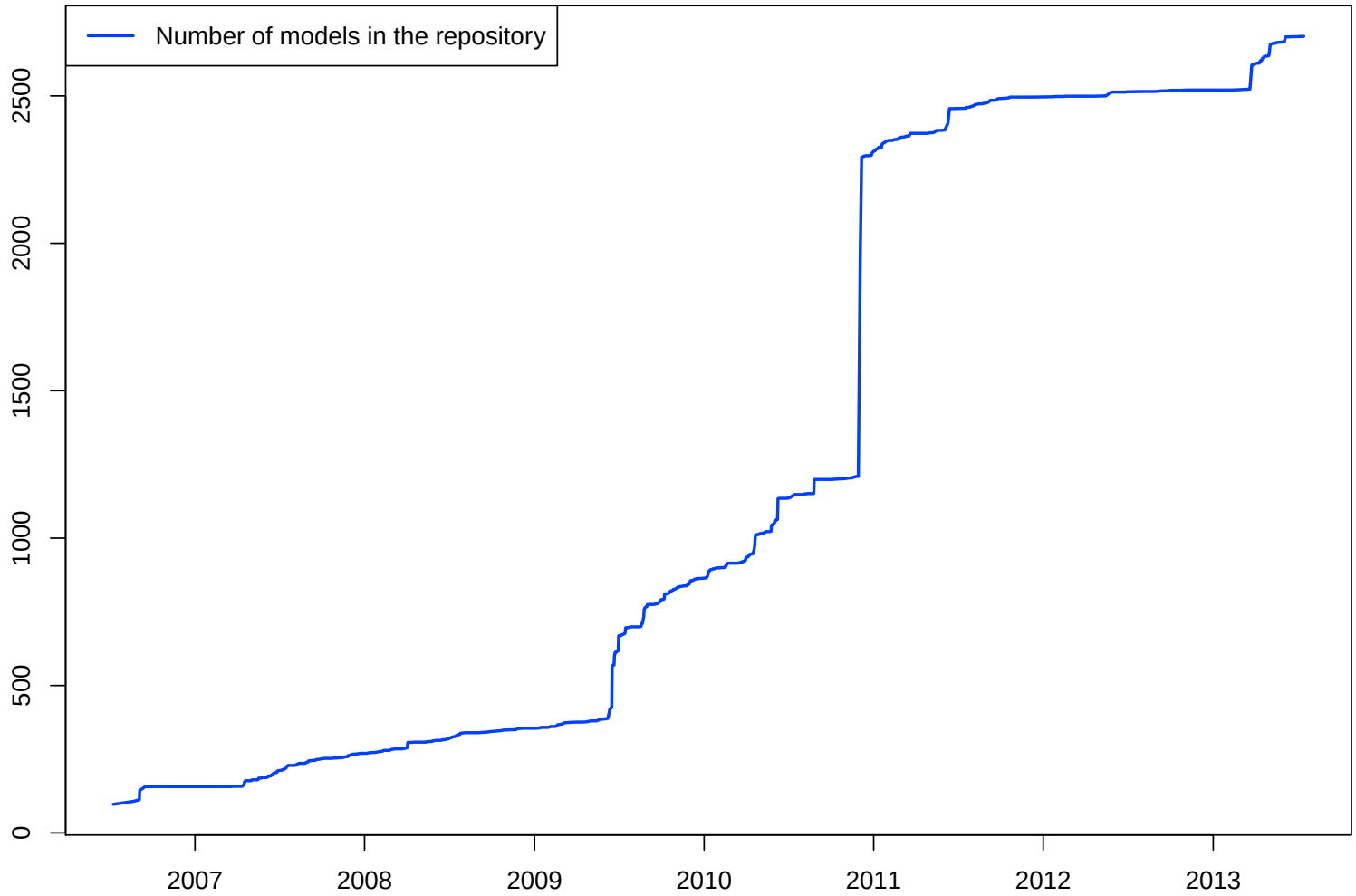
http://sems.uni-rostock.de

8th International CellML Workshop
Auckland, New Zealand 2014

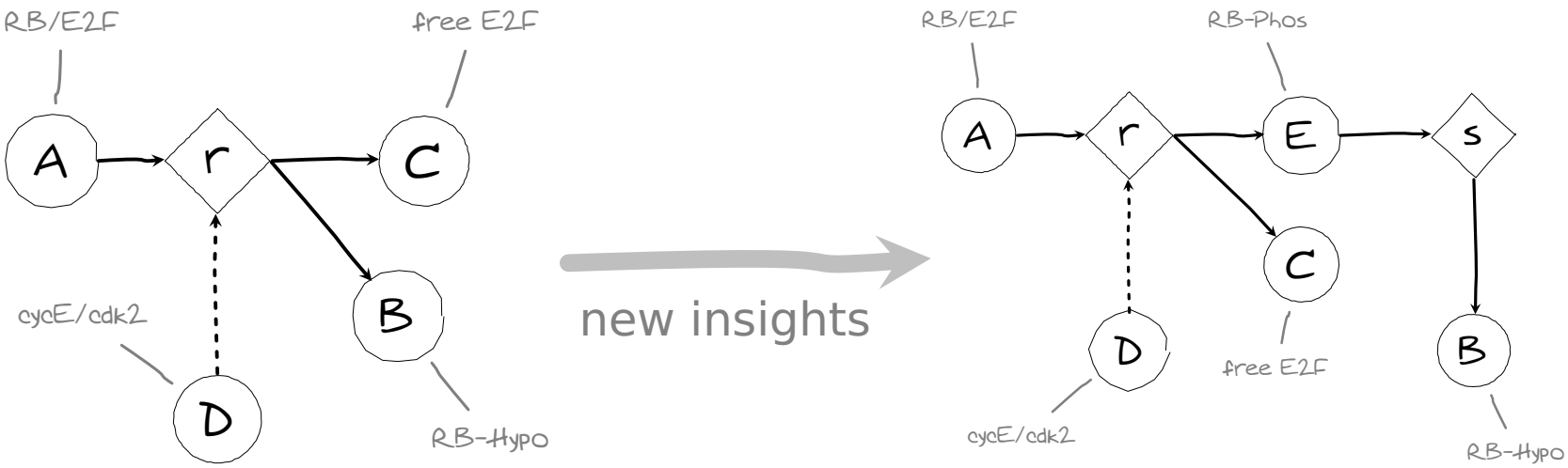


http://sems.uni-rostock.de/

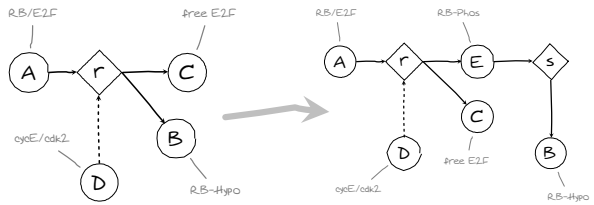
The CellML Model Repository



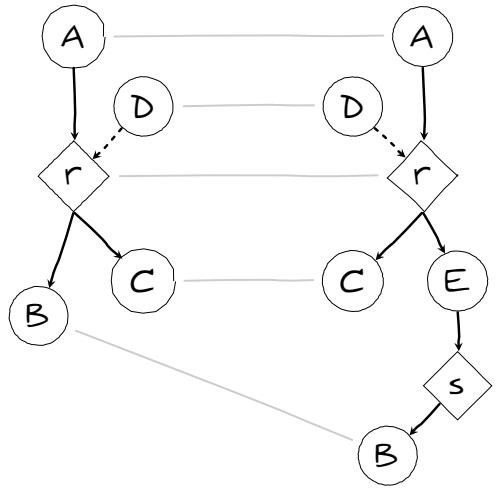
Version Control
good news



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



mapping

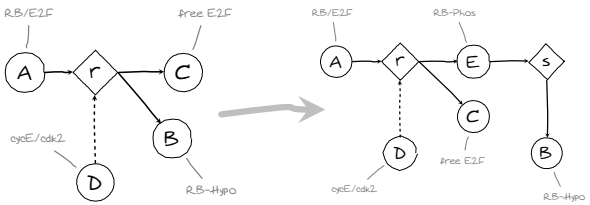


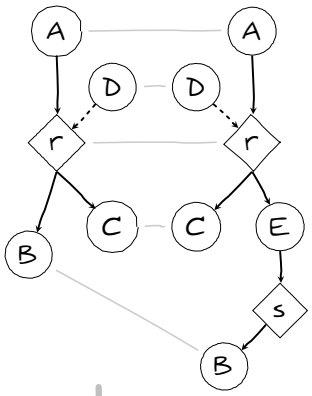
diff construction

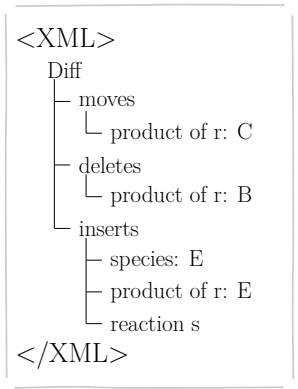
```
<XML>
  Diff
    moves
      product of r: C
    deletes
      product of r: B
    inserts
      species: E
      product of r: E
      reaction s
</XML>
```

Biochemical Model **Ve**rsion Control **S**ystem

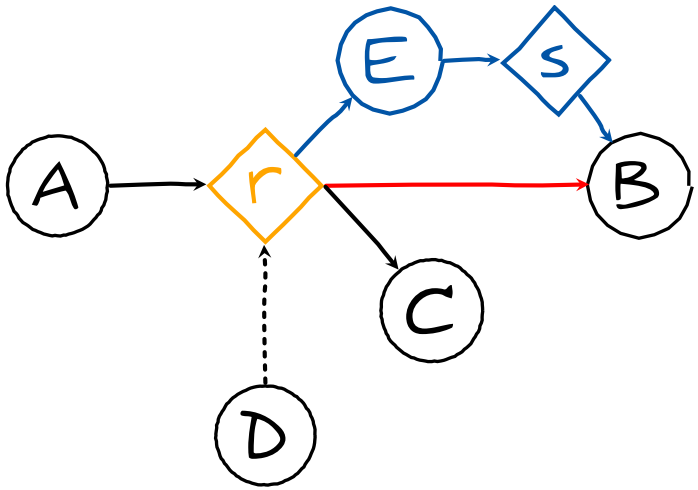
- compares models encoded in standadized formats (currently: SBML and CellML)
- maps hierarchically structured content
- constructs a delta (in XML format)
- is able to interprete this diff







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



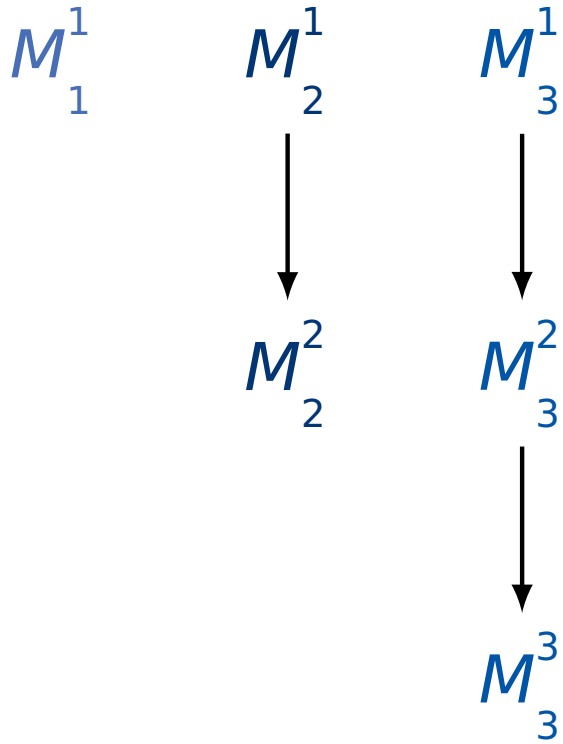
The CellML Model Repository

CellML Files 2702

```
for r in $repositories
do
     hg clone $r
done
```

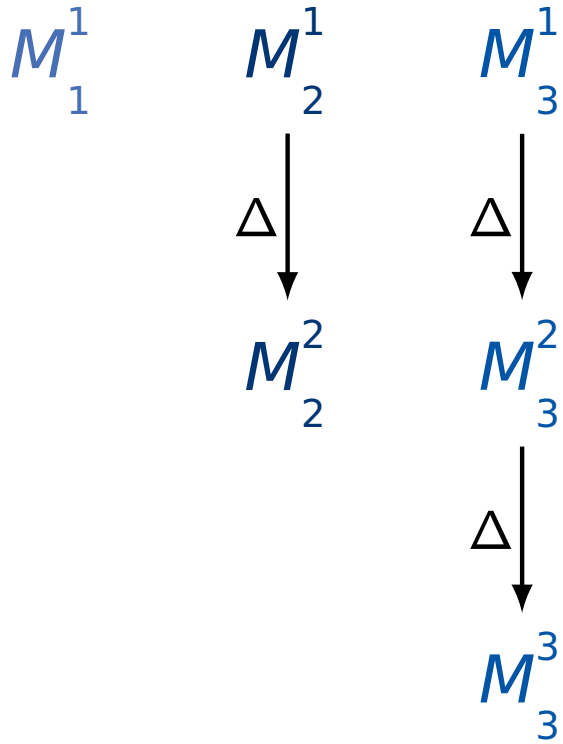
The CellML Model Repository

CellML Files 2702
Versions 18329



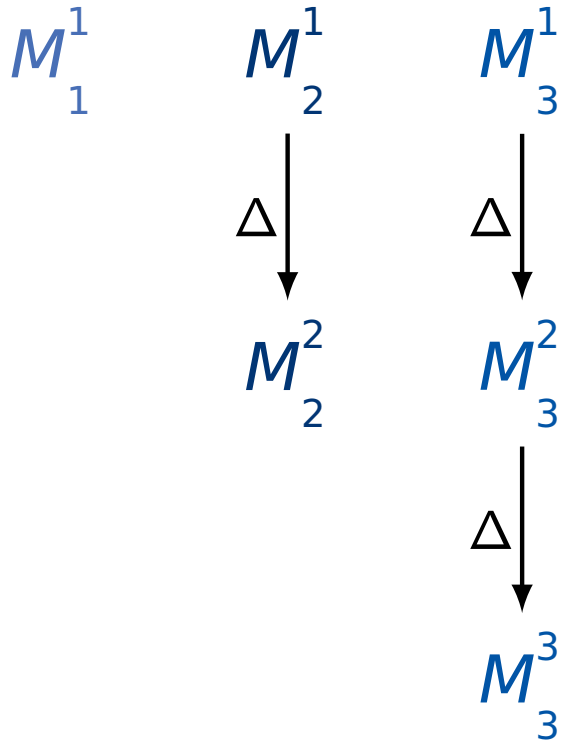
The CellML Model Repository

CellML Files	2702
Versions	18329
#Deltas	15626



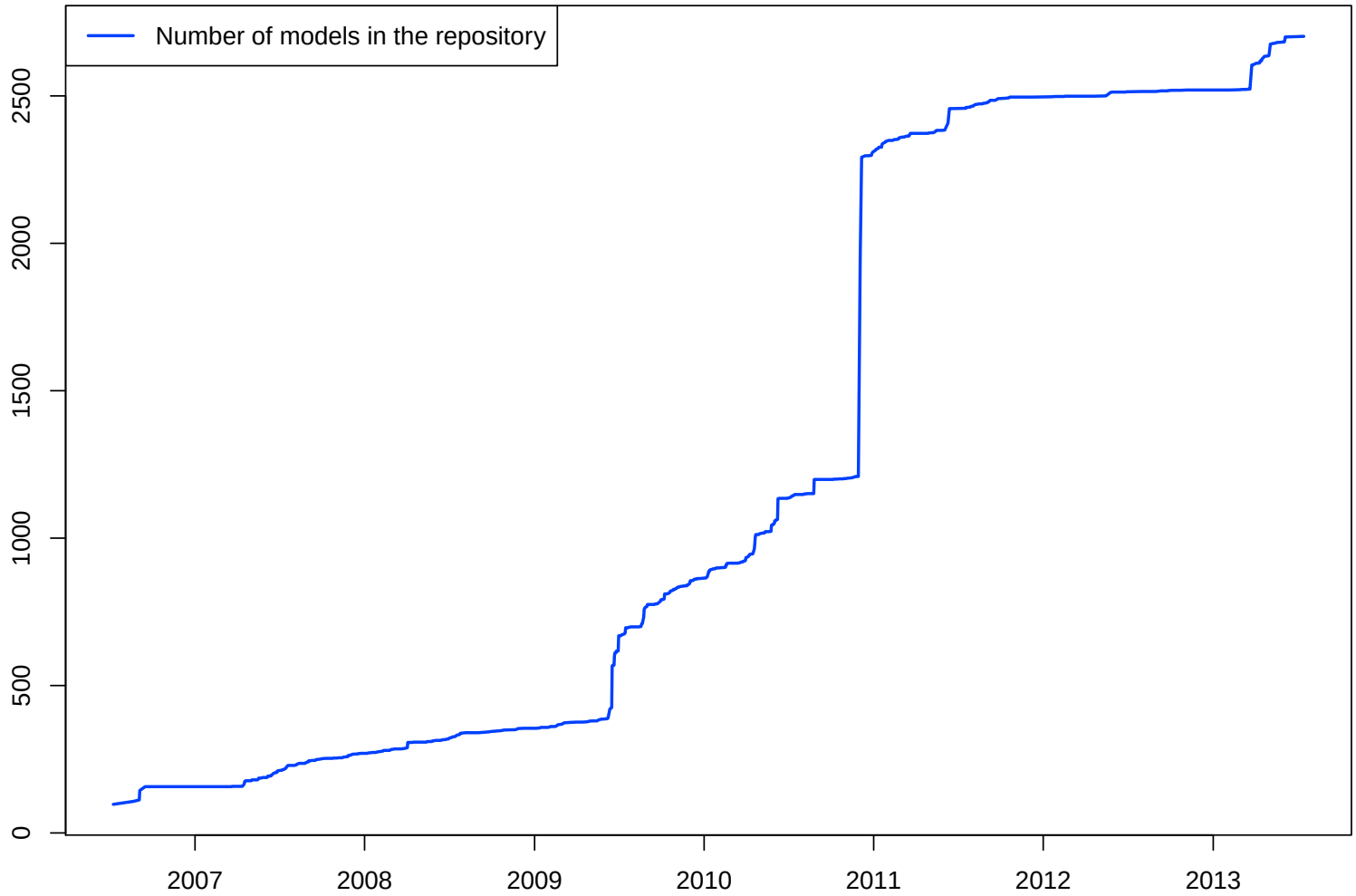
The CellML Model Repository

CellML Files	2702
Versions	18329
#Deltas	15626
#relevant	2833
∅#operations	355.31



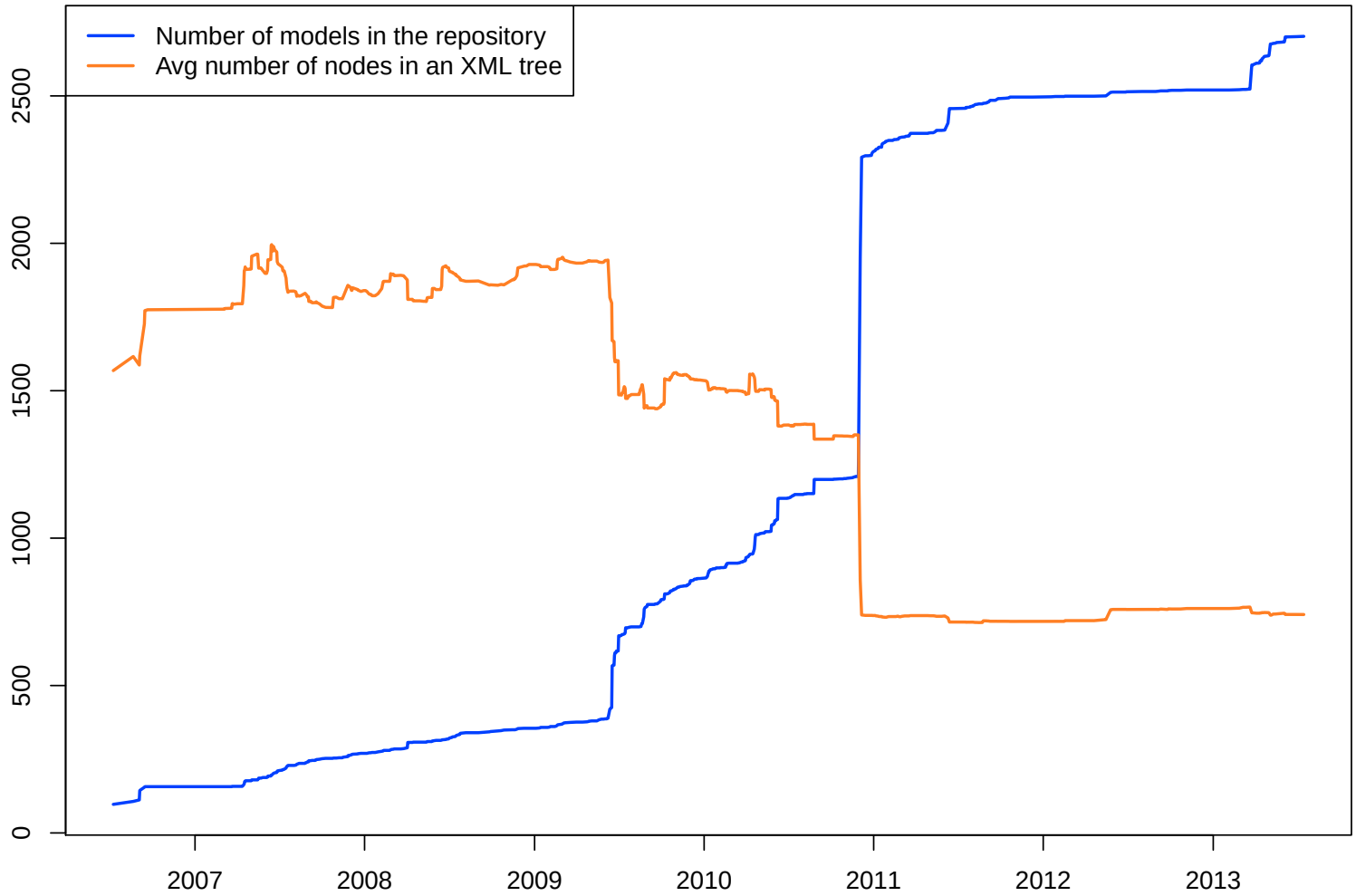
The CellML Model Repository

Growth



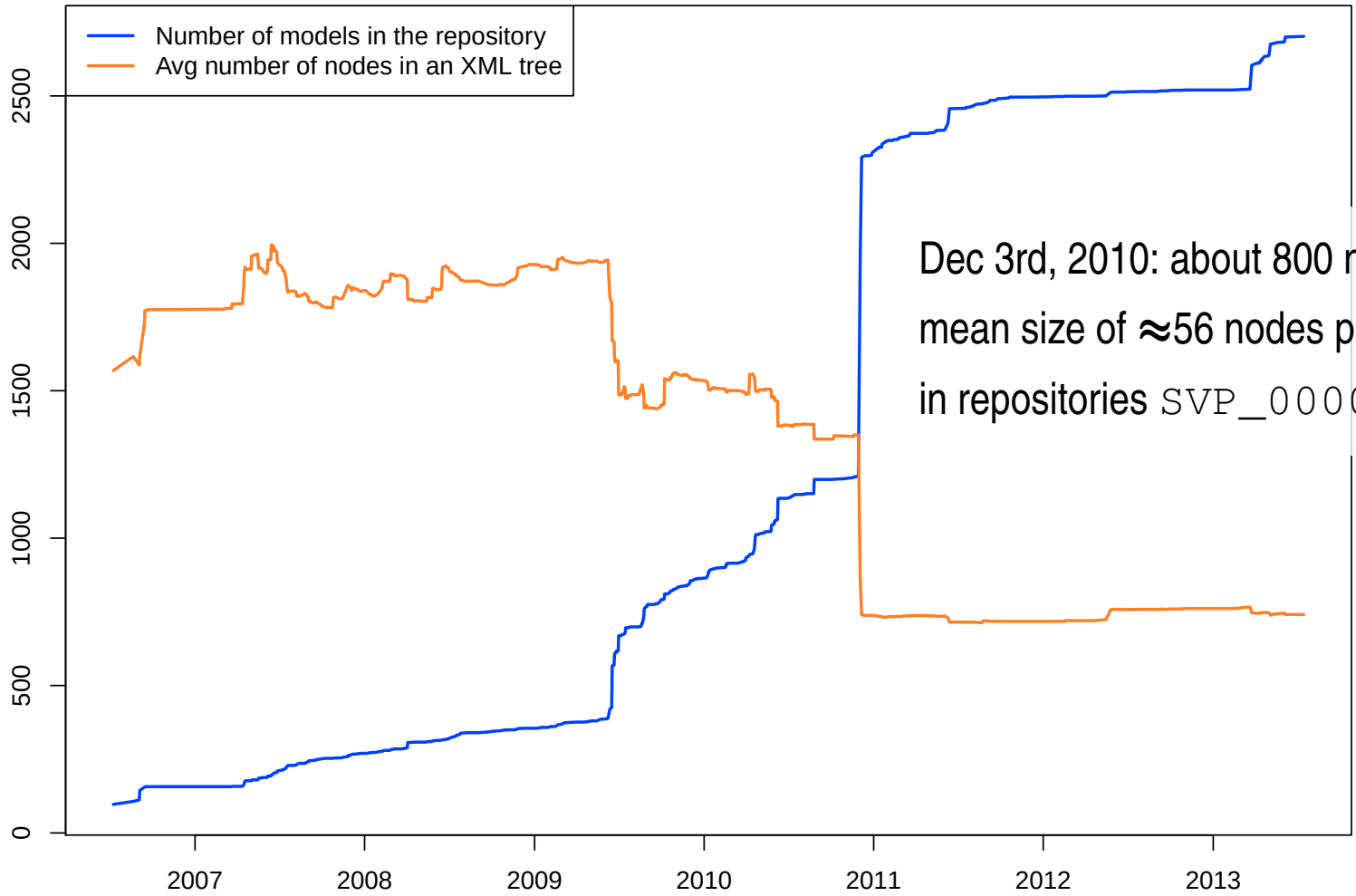
The CellML Model Repository

Growth



The CellML Model Repository

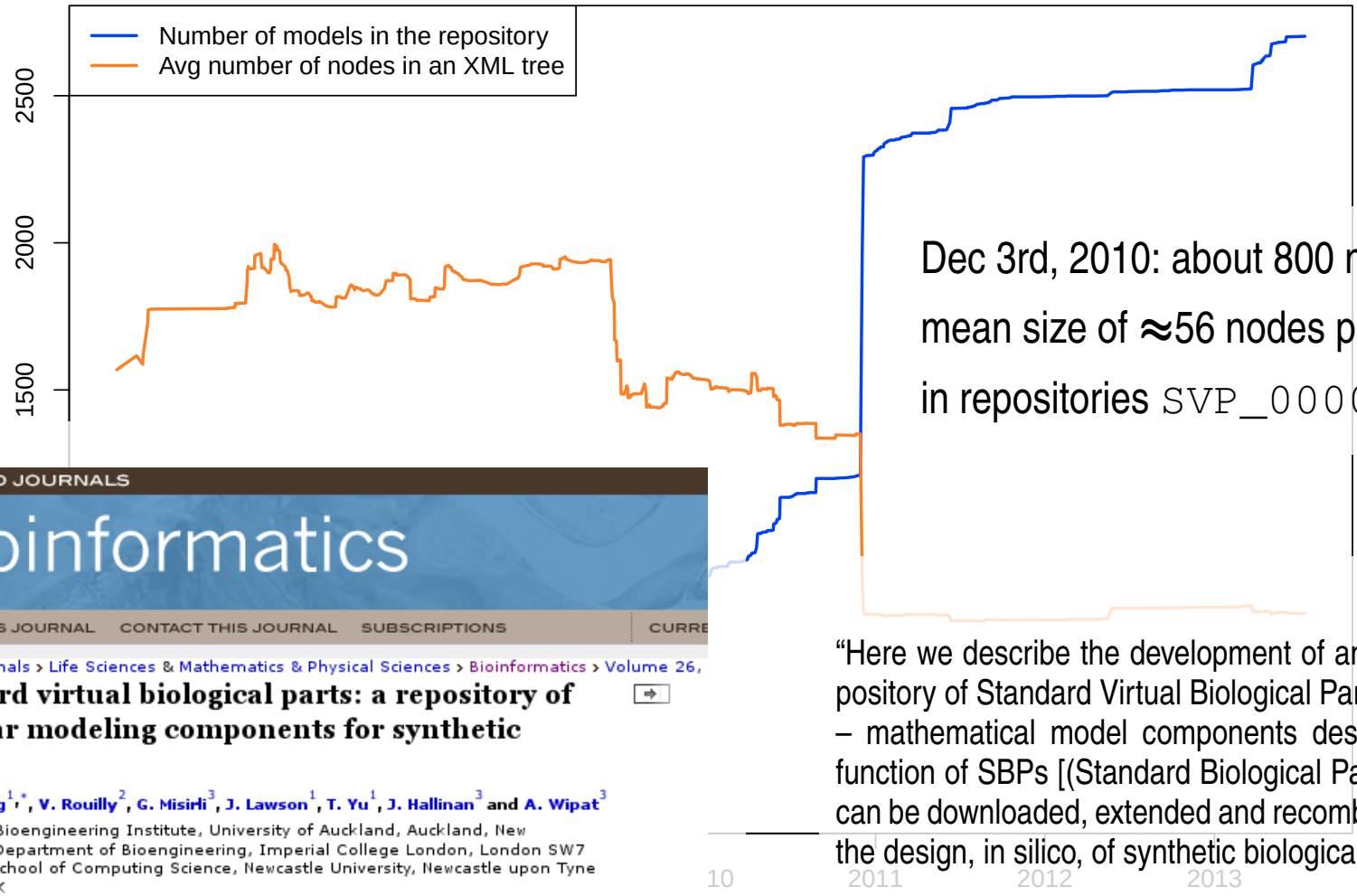
Growth



Dec 3rd, 2010: about 800 models with mean size of ≈56 nodes per model in repositories `SVP_0000*`

The CellML Model Repository

Growth



Dec 3rd, 2010: about 800 models with mean size of ≈56 nodes per model in repositories `SVP_0000*`

OXFORD JOURNALS

Bioinformatics

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Oxford Journals › Life Sciences & Mathematics & Physical Sciences › Bioinformatics › Volume 26,

Standard virtual biological parts: a repository of modular modeling components for synthetic biology

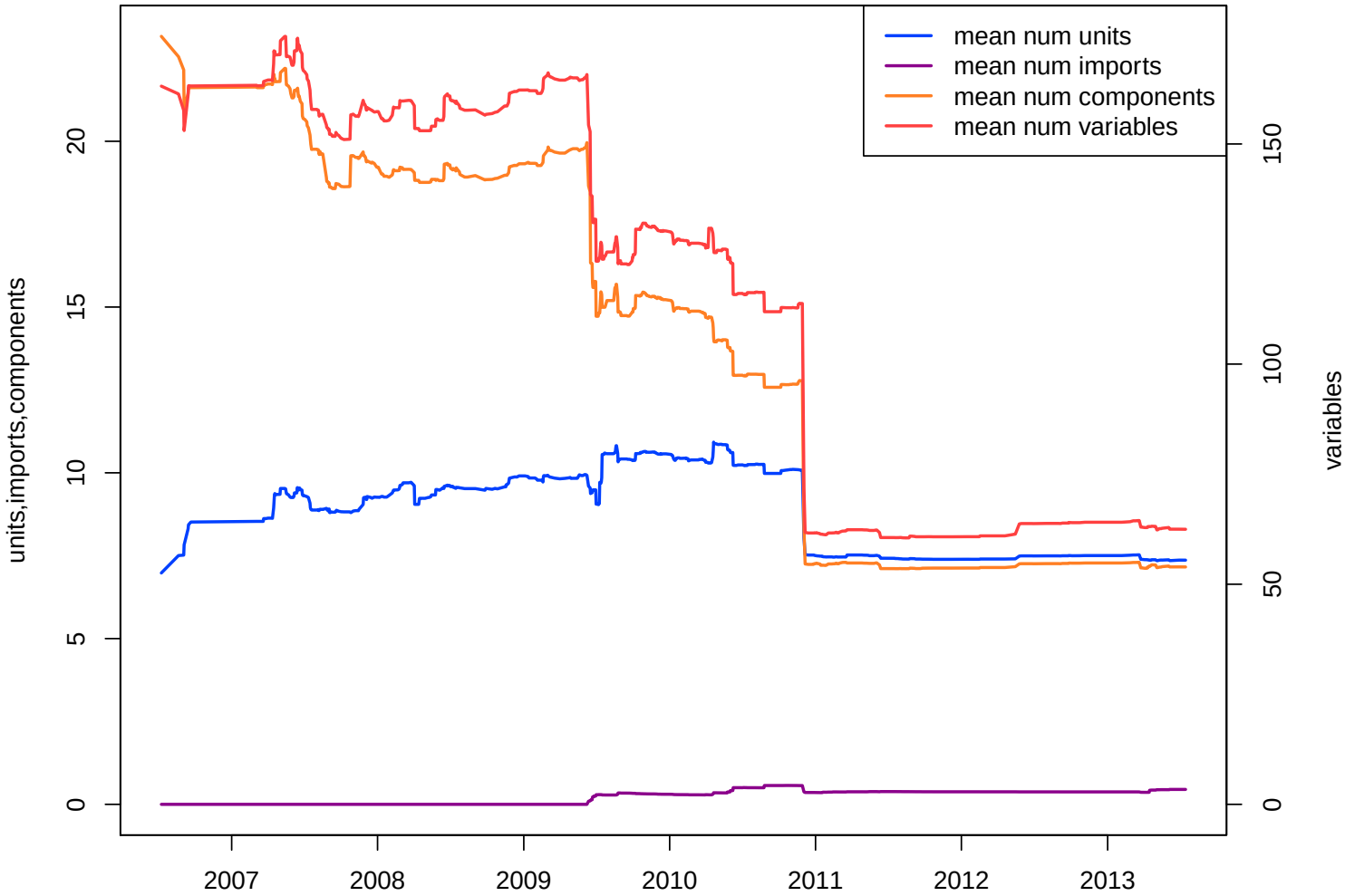
M. T. Cooling[1,*], V. Rouilly[2], G. Misirli[3], J. Lawson[1], T. Yu[1], J. Hallinan[3] and A. Wipat[3]

[1] Auckland Bioengineering Institute, University of Auckland, Auckland, New Zealand, [2] Department of Bioengineering, Imperial College London, London SW7 2AZ and [3] School of Computing Science, Newcastle University, Newcastle upon Tyne NE1 7RU, UK

"Here we describe the development of an online repository of Standard Virtual Biological Parts (**SVP**s) – mathematical model components describing the function of SBPs [(Standard Biological Parts)] which can be downloaded, extended and recombined to aid the design, in silico, of synthetic biological systems."

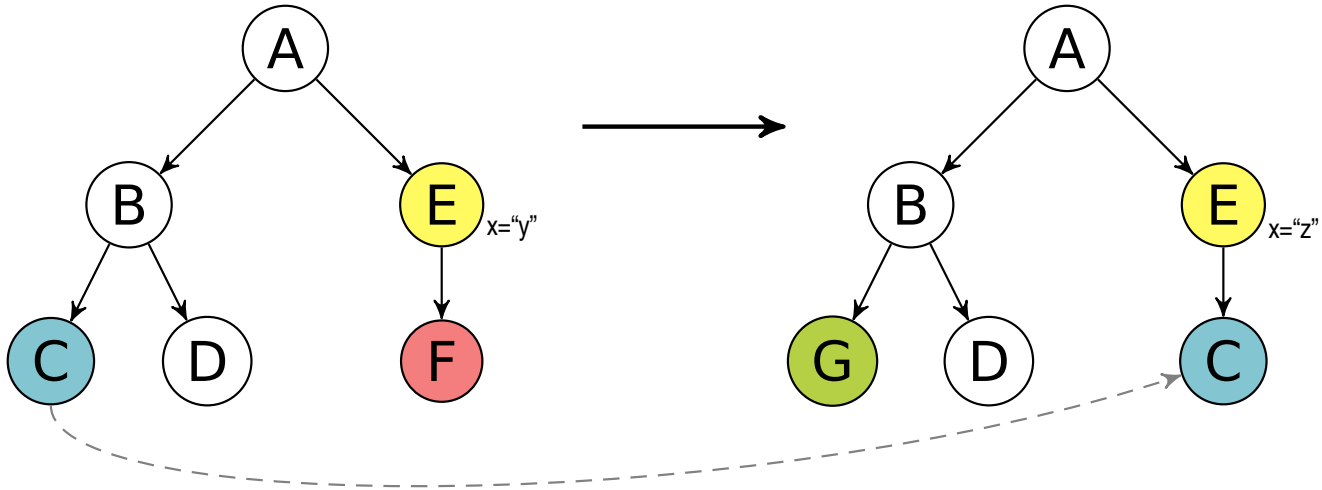
The CellML Model Repository

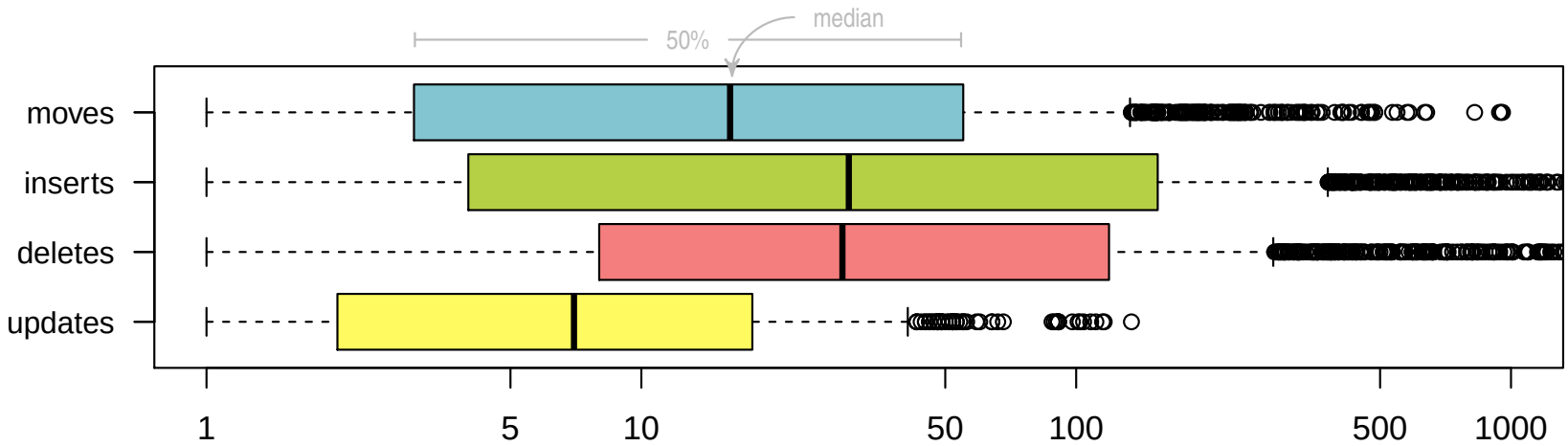
Growth



The CellML Model Repository

Types of Operation

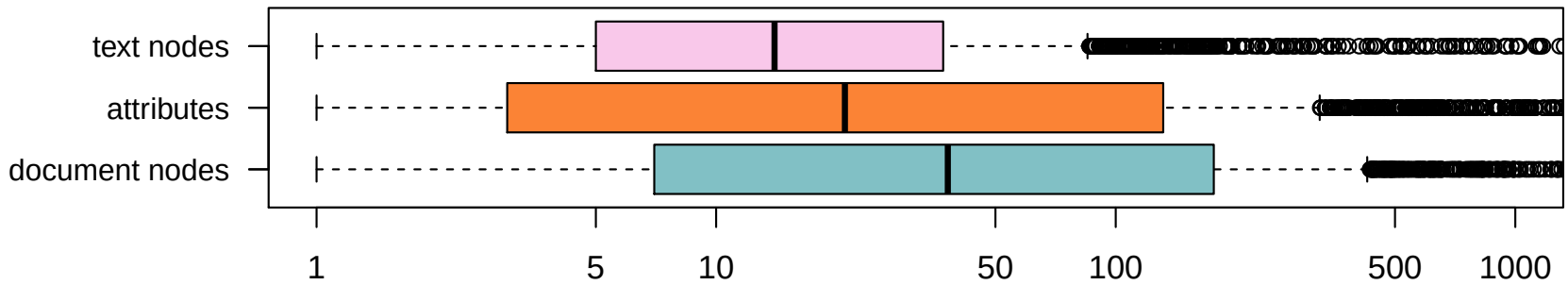




The CellML Model Repository

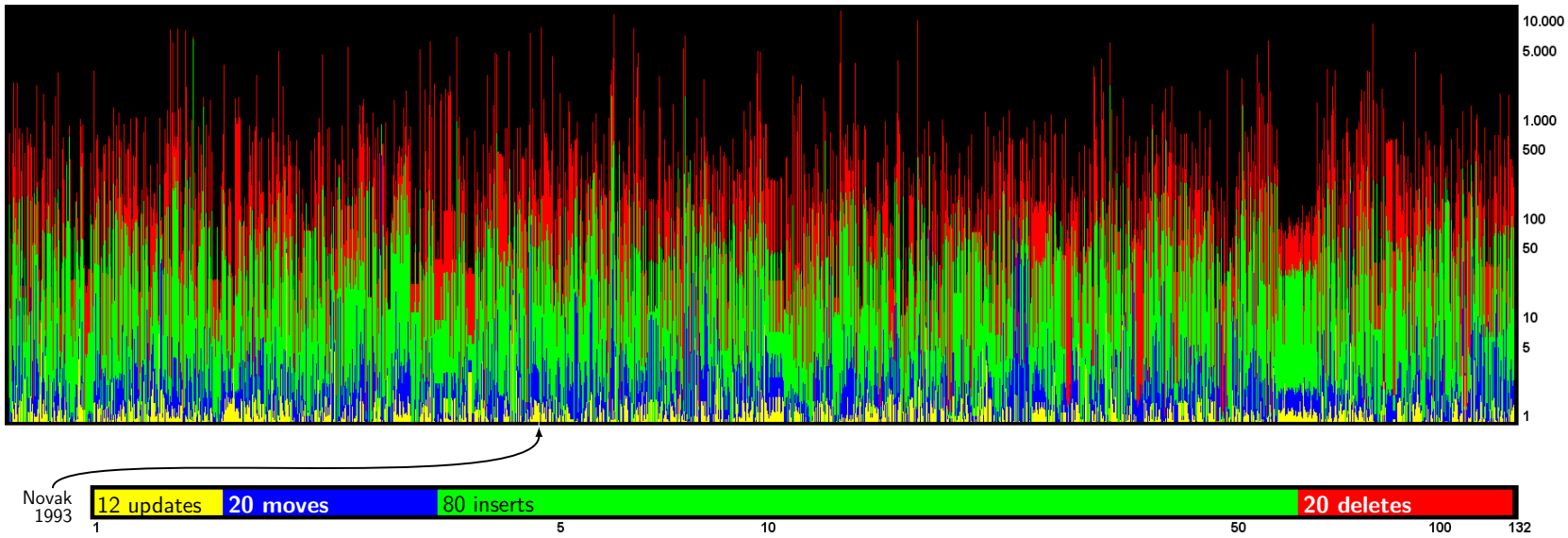
Modification Targets

```
<component name="Template_Species">
     <variable name="time" units="second" public_interface="in"/>
     <variable name="concentration" units="nM" initial_value="concInit" public_interface="out"/>
     <variable name="JGain" units="nM_per_s" public_interface="in"/>
     <math xmlns="http://www.w3.org/1998/Math/MathML">
          <apply>
               <eq/>
               <apply>
                    <diff/>
                    <bvar>
                         <ci>time</ci>
                    </bvar>
                    <ci>concentration</ci>
               </apply>
               <ci>JGain</ci>
          </apply>
     </math>
</component>
```



The CellML Model Repository

Operations



Thank you for your attention!

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für Bildung
und Forschung