



The COMBINE archive and the CombineArchive Toolkit

e:Bio Statusseminar



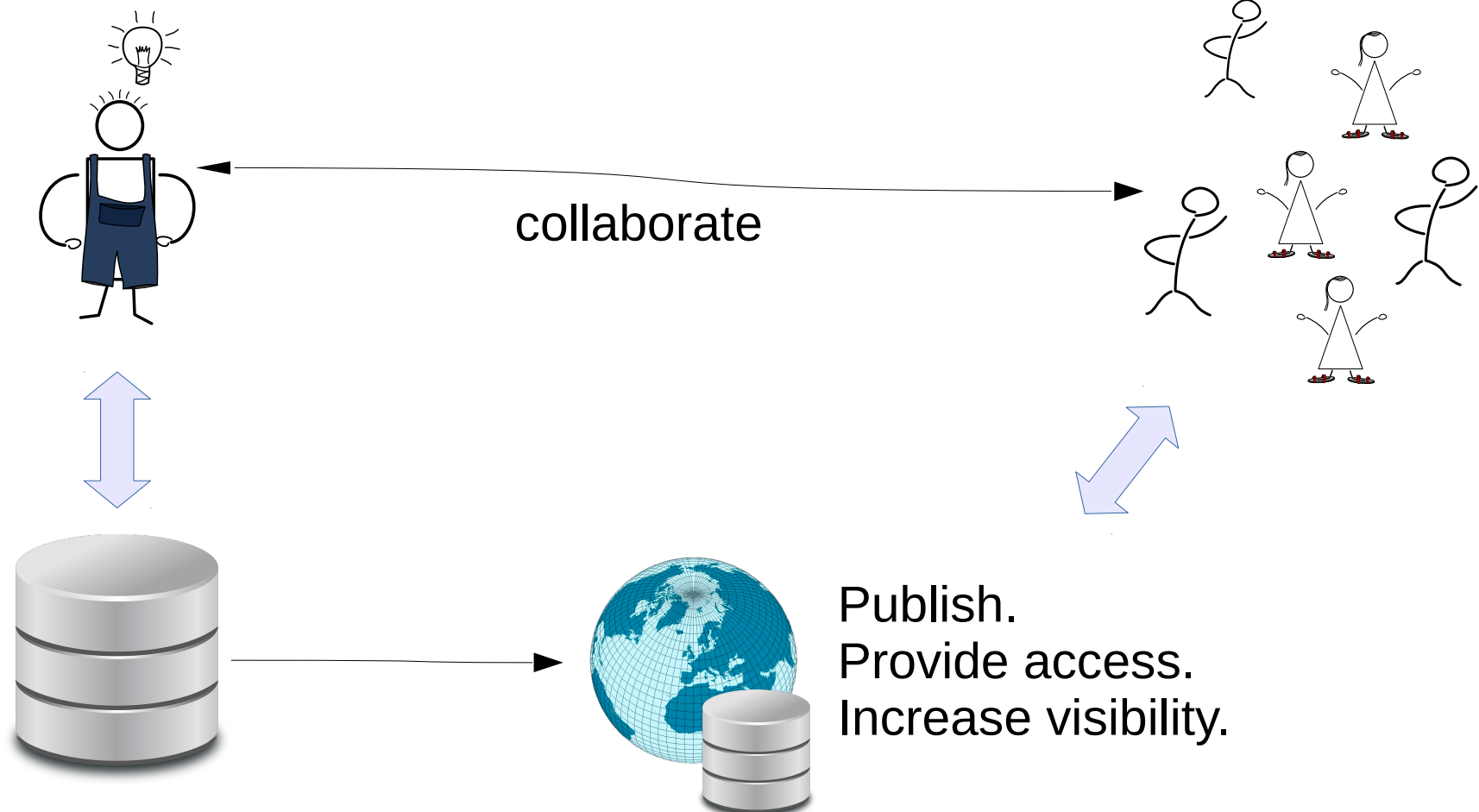
Berlin, 23rd of September 2014

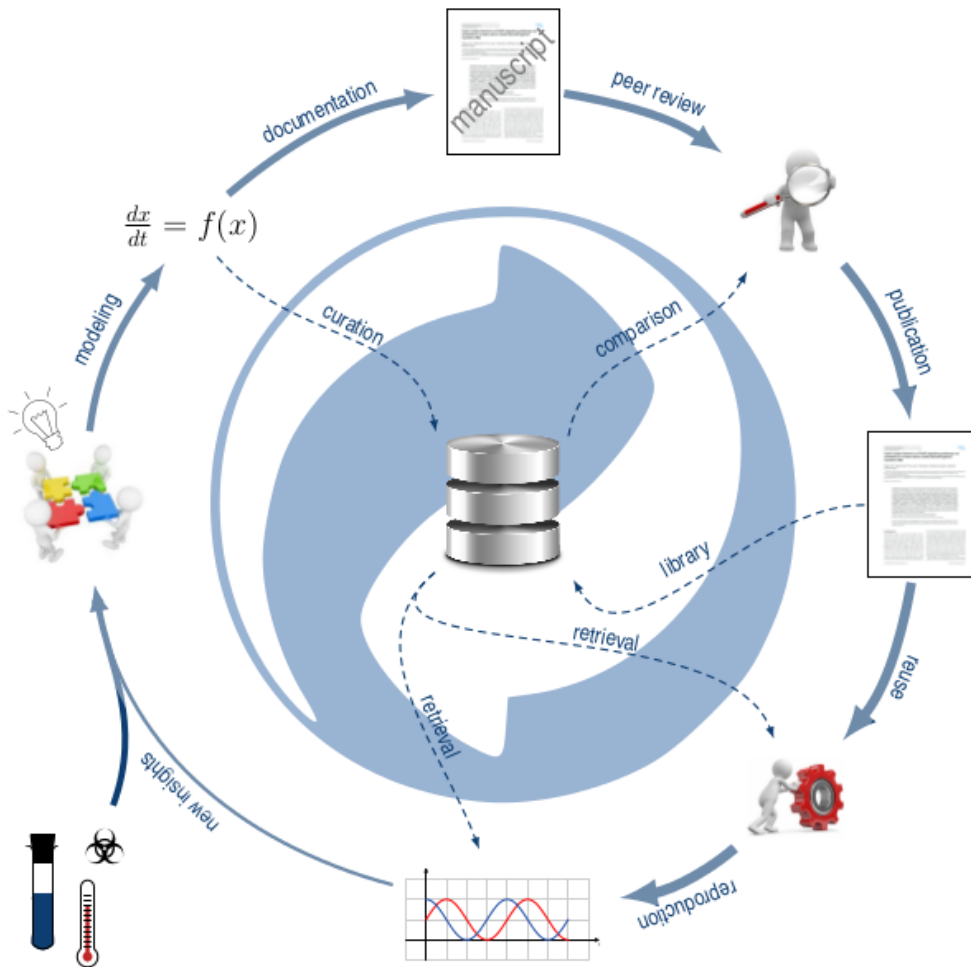
*SEMS – Managing Modeling Results in Systems Biology
Department of Systems Biology and Bioinformatics, University of Rostock*

Dagmar Waltemath, Martin Scharm, Olaf Wolkenhauer



Scientists share data.





Data in Systems Biology

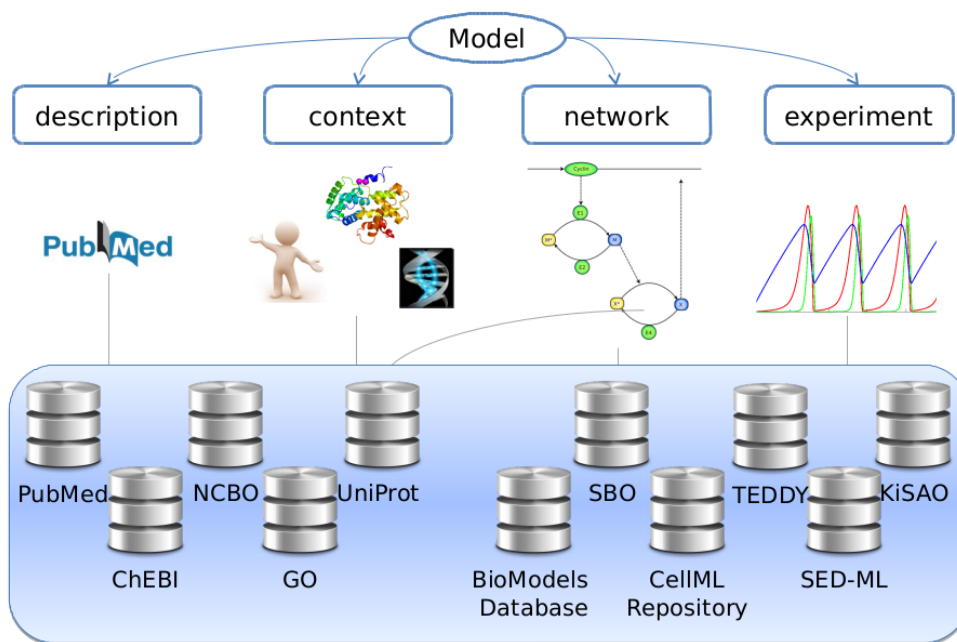
heterogeneous | distributed

standardised

... and often not reproducible

Figure courtesy Martin Scharm

Management of modeling results



Model version control

Waltemath et al (2013) Bioinformatics

Linking model-related data

Henkel et al (2014) PeerJ

Features for SBML model sets

Alm et al (2014) DILS

Standardization

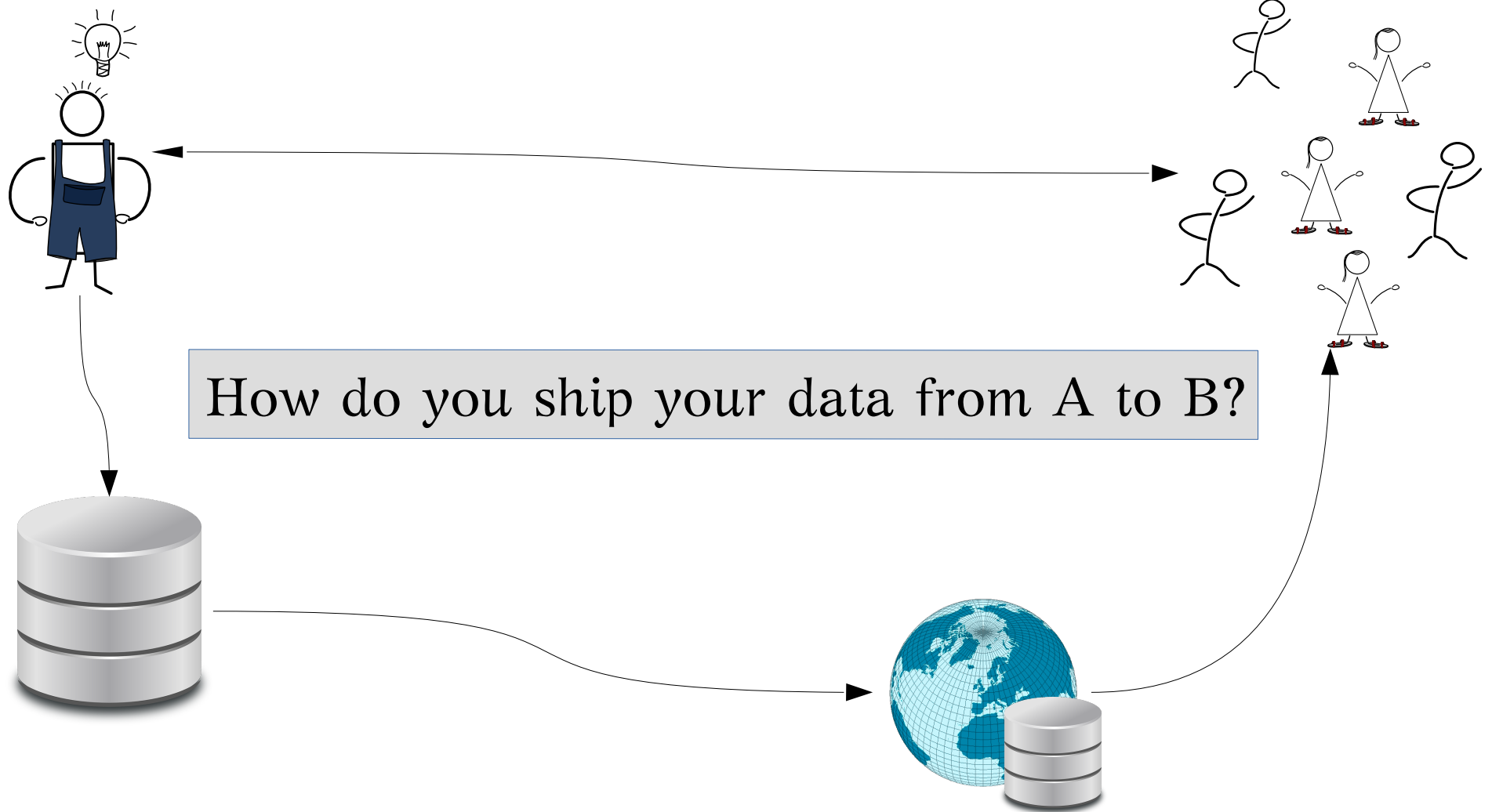
SBML, SED-ML, OMEX

Reproducibility of modeling results

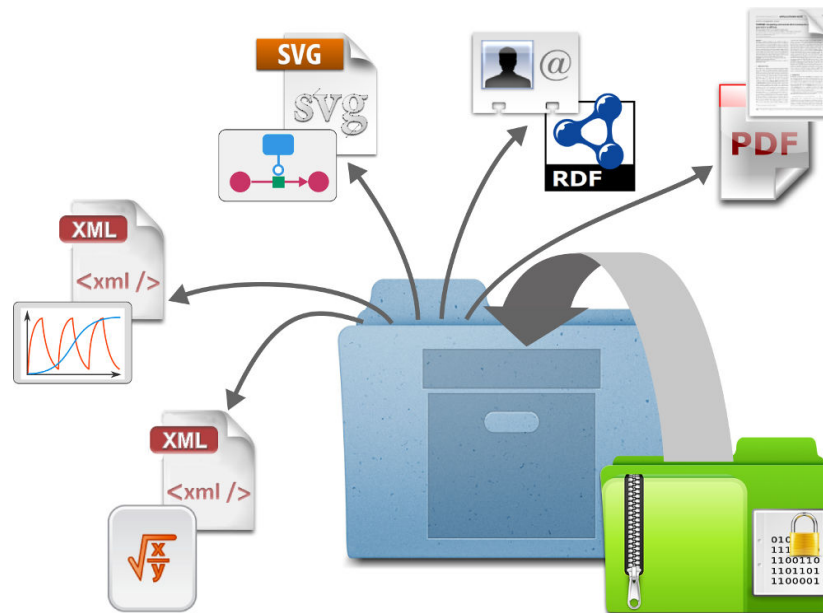
Waltemath et al (2013) Systems Biology

Defining virtual experiments

Cooper et al (2014) PeerJ



The COMBINE Archive



arXiv.org > cs > arXiv:1407.4992

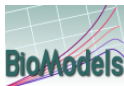


Search or Article-Id

Computer Science > Digital Libraries

COMBINE archive: One File To Share Them All

Frank T. Bergmann, Richard Adams, Stuart Moodie, Jonathan Cooper, Mihai Glont, Martin Golebiewski, Michael Hucka, Camille Laibe, Andrew K. Miller, David P. Nickerson, Brett G. Olivier, Nicolas Rodriguez, Herbert M. Sauro, Martin Scharm, Stian Soiland-Reyes, Dagmar Waltemath, Florent Yvon, Nicolas Le Novère

The COMBINE Archive

- .zip file (**O**pen **M**odeling **EX**change Format)
- Content:
 - Manifest.xml – location and type of each file in the archive
 - Metadata files – with clerical information
 - The files – necessary to reproduce a modeling result
- Supported by  ,  , 

The COMBINE Archive

```
<?xml version="1.0" encoding="utf-8"?>
<omexManifest xmlns="http://identifiers.org/combine.specifications/omex-manifest">
  <content location="."
    format="http://identifiers.org/combine.specifications/omex"/>
  <content location="models/model.xml"
    format="http://identifiers.org/combine.specifications/sbml"/>
  <content location="simulation.xml" master="true"
    format="http://identifiers.org/combine.specifications/sed-ml"/>
  <content location="doc/article.pdf"
    format="http://purl.org/NET/mediatypes/application/pdf"/>
  <content location="metadata.rdf"
    format="http://identifiers.org/combine.specifications/omex-metadata"/>
</omexManifest>
```

Bergmann et al. (2014) COMBINE Archive – One File To Share Them All (arxiv)

The COMBINE Archive Toolkit

- Java library
 - Extracting single files / whole archive
 - Browsing through the archive
 - Adding and removing files
 - Renaming and organising files
 - Attaching and retrieving meta data
- Desktop application
- Web interface



Martin Scharm



Florian Wendland



Martin Peters

CombineArchiveWeb

[start] [create]

::test ::biomd0000000459

id:83baa618-9870-4518-a455-86a8ebb6fa57
name: BIOMD0000000459

[Download] [Edit] [Delete]

UPLOAD FILES

Archive Content

[New folder]

- BIOMD0000000459-SEDML.xml
- BIOMD0000000459.xml
- liebal2012.pdf
- MODEL1302080001.png

BIOMD0000000459 - SEDML.xml

file name: BIOMD0000000459-SEDML.xml
file path: /BIOMD0000000459-SEDML.xml
format: http://identifiers.org/combine.specifications/sedml
size: 3.76 KB
master: no

[Add OMEX meta] [Download] [Edit] [Delete]

OMEX entry

created: 6/6/2013, 7:26:06 PM
modified: [6/10/2013, 1:51:33 PM]
[7/7/2014, 4:50:01 PM]
creators:
given name: Ulf
family name: Liebal
E-Mail: ulf.liebal@uni-rostock.de
organization: University of Rostock
given name: Markus
family name: Wolfien
E-Mail: markus.wolfien@uni-rostock.de
organization: University of Rostock

[Edit] [Delete]



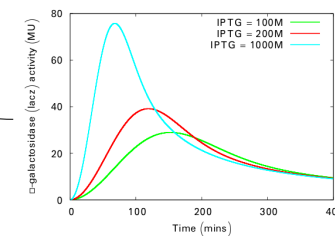
```
<?xml version="1.0" encoding="UTF-8" ?>
<!-- Created by COPASI version 4.10.0 -->
<sbml xmlns="http://www.sbml.org/sbml/2002" level="3" version="3" >
  <model metaid="COPASI1" >
    <notes>
```



Proteolysis of beta-galactosidase following SigmaB activation in *Bacillus subtilis*†

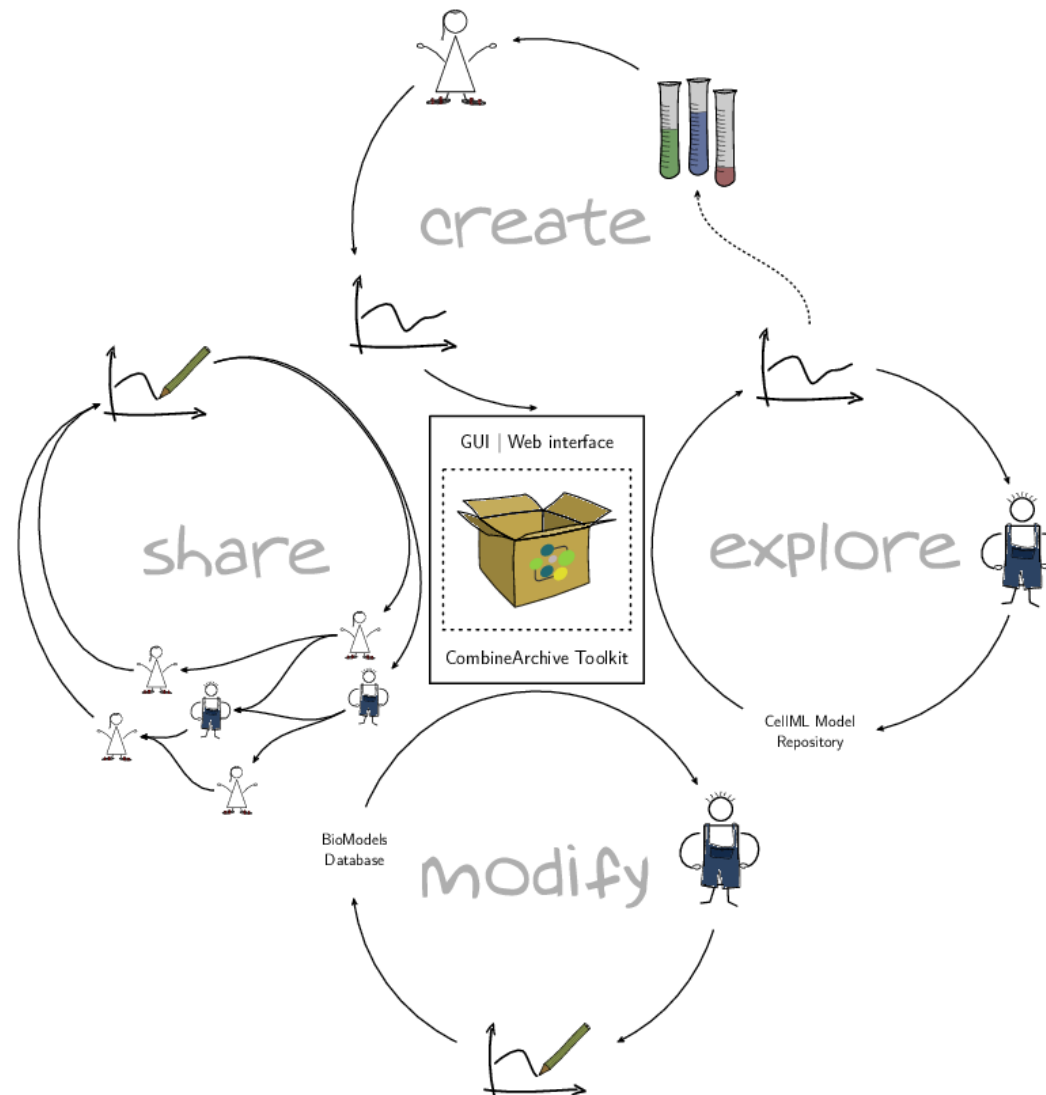
Ulf W. Liebal,^{†,*,a} Praveen K. Sappa,^{†,b} Thomas Millat,^a Leif Steil,^b Georg Homuth,^b Uwe Völker,^b and Olaf Wolkenhauer^{ac}

Received 25th January 2012, Accepted 20th March 2012
DOI: 10.1039/c2mb25031d



```
<?xml version="1.0" encoding="UTF-8" ?>
<!-- Written by libSedML -->
<sedML level="1" version="1" >
  <listOfSimulations>
    <uniformTimeCourse id="1" >
      <algorithm kisaoID="1" >
```

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



Scharm et al. (2014) submitted to SWAT4LS, Dec 9-10, Berlin



SEMS

Martin Scharm
Martin Peters
Markus Wolfien
Olaf Wolkenhauer

Associated members

Ron Henkel
Rebekka Alm
CAT Team



VolkswagenStiftung

Whole-cell modeling
summer school

March 9-13, 2015
Rostock, Germany



This work is licensed under the [CC BY-NC-ND 4.0](http://creativecommons.org/licenses/by-nc-nd/4.0)

