

# Minimum Information About a Simulation Experiment (MIASE)

- Toward the Repetition of Simulation Runs

Dagmar Köhn, Nicolas Le Novère



# MIASE

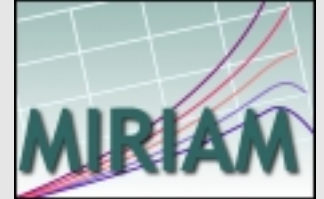
“The aim of MIASE is to provide all the information necessary to link a model to a set of numerical results, in order to reproduce the latter.”

## Outline:

- Motivation for MIASE
- Project description
- A first approach – MIASE

# MIASE – Motivation: MIRIAM

## MIRIAM – Minimum Information Requested In the Annotation of biochemical Models



- Aim:
  - standardization effort for the annotation of models in order to provide a more effective (and standardized) characterization to allow them to be re-used
- Problem:
  - “The model, when instantiated within a suitable simulation environment, must be able to reproduce all relevant results given in the reference description that can readily be simulated”
  - but: MIRIAM does not include guidelines about how a relevant result can be reproduced

# MIASE – Motivation: BioModels Database

- repository for biological models in SBML format
- Aims
  - researchers should be able to **exchange and share their results**
- Problem
  - most models are supplied as **plain SBML** code
  - a “model curator” does not have any information about simulation settings that led to the validation of the supplied model
  - after curation, the model is made available on biomodels.net, including a **screenshot** of the validated model
  - the next user has to **re-do the whole process** of identifying parameter settings before he/she can use the model
- Solution:
  - Provide **information about the simulation settings** in line with the model suppliance

# MIASE – Motivation: BioModels Database

**Reference Publication**

Publication ID: [12691603](#)

Biochem J 2003 Jul;373(Pt 2):451-63.  
A computational model on the modulation of mitogen-activated protein kinase (MAPK) and Akt pathways in heregulin-induced ErbB signalling.  
Hatakeyama M, Kimura S, Naka T, Kawasaki T, Yumoto N, Ichikawa M, Kim JH, Saito K, Saeki M, Shirouzu M, Yokoyama S, Konagaya A.  
RIKEN Genomic Sciences Center, 1-7-22 Suehirocho, Tsurumi-ku, Yokohama, Kanagawa 230-0045, Japan.  
marikoh@gsc.riken.go.jp [\[more\]](#)

**Model**

<b>Original Model:</b> <i>Unspecified</i>	bqbiol:is	set #1	<a href="#">Taxonomy</a> <a href="#">Cricetinae</a>
<b>Submitter:</b> <a href="#">Nicolas Le Novere</a>	bqbiol:isVersionOf	set #1	<a href="#">Gene Ontology</a> <a href="#">regulation of MAPK activity</a> <a href="#">Gene Ontology</a> <a href="#">regulation of protein kinase B signaling cascade</a>
<b>Submission Date:</b> 2007-09-06T09:06:00			
<b>Last Modification Date:</b> 2007-09-21T20:59:42			

<http://www.ebi.ac.uk> - Simulation Res

**Simulation Result**

Time (s) vs R.P. (%)

Time (s)	R.P. (%)
0	80
250	45
500	40
750	35
1000	30
1250	28
1500	25
1750	22

Done

[Simulation Result](#) | [GIF Reaction Graph](#) | [SVG Reaction Graph](#) | [Dynamic Reaction Graph](#)

**Simulation Tool**

**Re-Create**

Compartments (1)  
Species (33)  
Rules (7)  
Events (0)

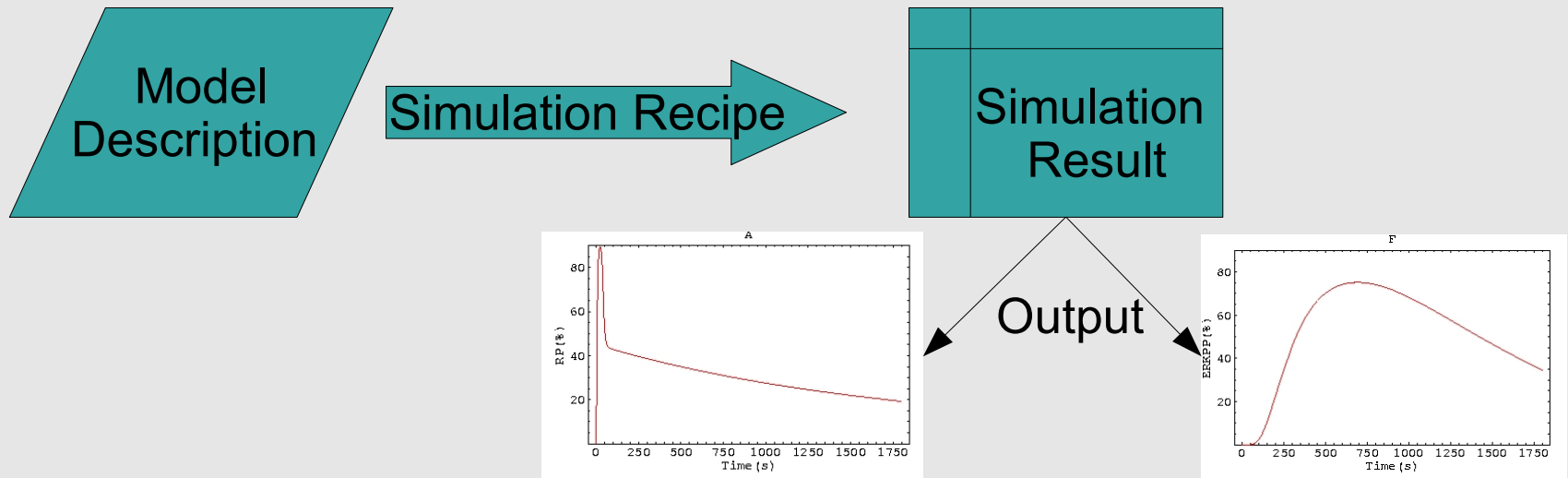
# MIASE – Project Description

The project is split into three parts:

- MIASE guidelines
  - Textual description of the meta-data necessary to describe simulation runs
- Data Model
  - Formal description of guidelines
  - Data model representation in XML Schema, ... ?
- Simulation Algorithm Ontology for Biochemical Simulation Experiments (KiSAO)
  - Main simulation algorithms and their classification

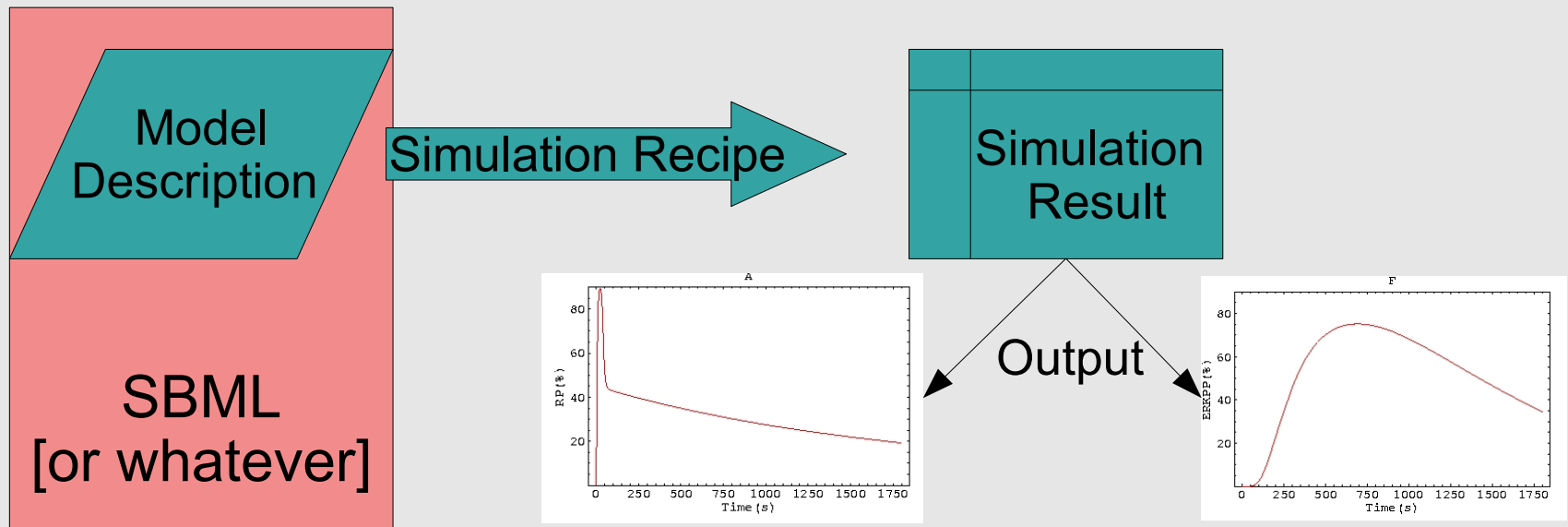
# MIASE

- MIASE should cover the minimum information about a simulation experiment
  - Simulation tool
  - Time scale & iteration procedure
  - Set of parameters to scan
  - Sampling method ...



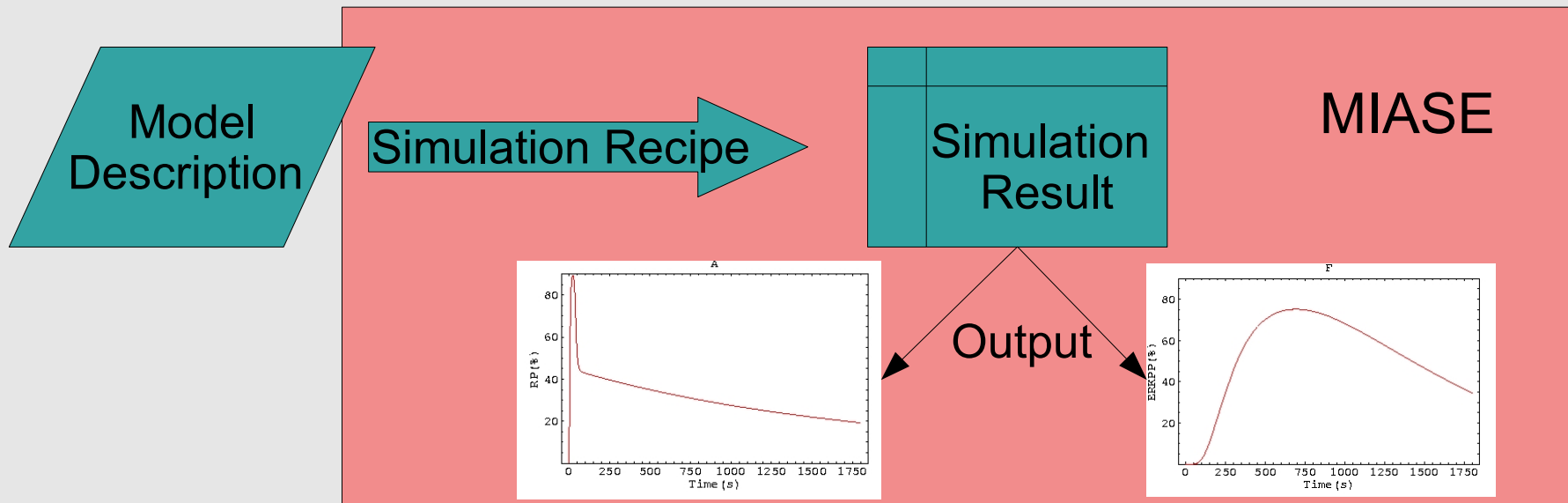
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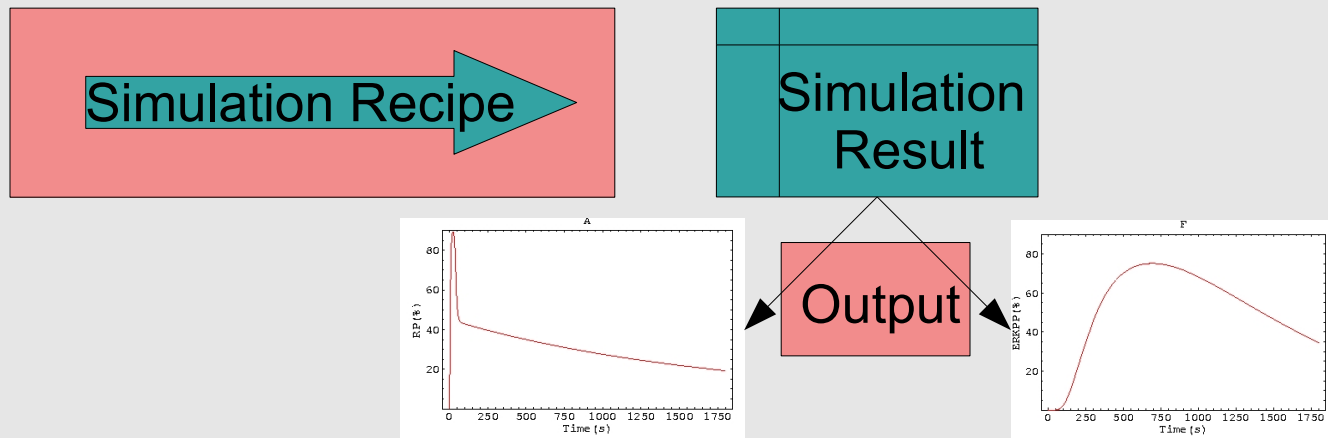
# MIASE

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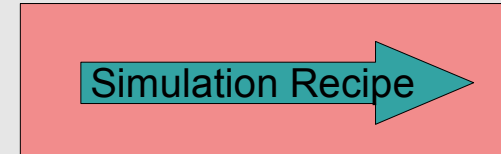
# MIASE

- Identifying MI for the repetition of simulation runs
- Tasks
  - (1) Identify MI for SBML models stored in BioModels Database and simulated in COPASI
  - (2) Find a more generic solution
- Information encoded in MIASE
  - Information on the simulation
  - Information on the output



# MIASE

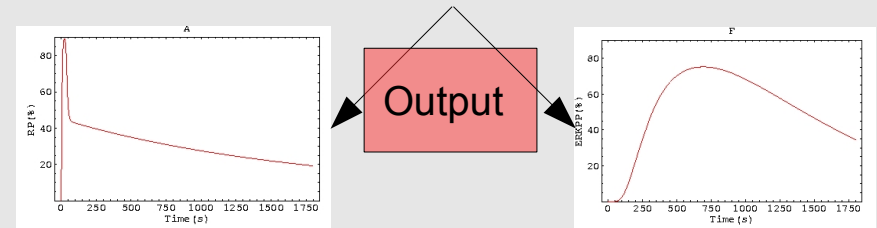
- Information on the simulation
  - ModelID
  - Simulation Tool used
  - Simulation Algorithm used (KiSAO)
  - Aim of the simulation (time course, steady state ...)
  - Depending on the simulation aim, additional information has to be provided, e.g.
    - for a time-course:
      - Type of simulation time used (real time, model time...)
      - Simulation duration (Simulation steps, interval)
    - for a parameter scan:
      - Scan interval
      - parameter scanned (ID as given in the model)



# MIASE

- Information on the output

- Type of output (2D/3D-graph, report...)
- Depending on the type of output, additional information has to be provided, e.g.
  - for a Graph:
    - Variables plotted on which axis (ID as given in the model)
    - Scales on the axes



# MIASE Data Model

The MIASE-DM will provide a formal representation of the minimum information description.

(not yet implemented)

```
<xs element name="plot">
  <xs:complexContent> <xs:sequence>
    <xs:element name="x-Axis" type="xs:string" />
    <xs:element name="y-Axis" type="xs:string" />
    <xs:element name="z-Axis" type="xs:string"
      use="optional" />
  </xs:sequence> </xs:complexContent>
</xs:element>
```

# We [still] need help :)

- discussion about the MI content
  - granularity of encoded information
  - how much information can be automatically extracted from the simulation tools?
  - ....
- Verification of the content

online resources and information:

- <http://sourceforge.net/projects/miase>
- <http://www.ebi.ac.uk/compneur-srv/miase>

contact:

- [lenov@ebi.ac.uk](mailto:lenov@ebi.ac.uk)
- [dagmar@ebi.ac.uk](mailto:dagmar@ebi.ac.uk)

# MIASE – Detailed description of the MI

- Reference to the according model
  - n:m relation
    - more than one models could be run using the same simulation settings (e.g. variants of the same model)
    - a model can be run using different settings
  - `<xs:element name="modelId" type="xs:string" minOccurs="1" />`

# MIASE – Detailed description of the MI

- Simulation tool used
  - refers to the simulation tool used for the simulation to be run
  - name and version
  - a result might have been achieved by using more than one simulation tool (concurrently or serially)s, that is why a list of tools should be provided

```
<xs:element name="simulationTool"
  type="simulationToolType" />
<xs:complexType name="simulationToolType">
<xs:complexContent><xs:sequence>
  <xs:element name="name" type="xs:string"/>
</xs:sequence> </xs:complexContent>
  <xs:attribute name="version" type="xs:string" />
</xs:complexType>
```

# MIASE – Detailed description of the MI

- General information about the simulation run
  - creator/author + institution

```
<xs:element name="simulationExperiment" type="MIASE" />
<xs:complexType name="MIASE">
  <xs:complexType>
    <xs:sequence>
      <xs:element name="simulator" type="xs:string" />
      ...
    </xs:sequence>
  </xs:complexType>
</xs:complexType>
```

# MIASE – Detailed description of the MI

- Aim of the simulation
  - what type of simulation has been done?
    - time course
    - steady state
    - stoichiometry
    - metabolic control analysis
    - ...

# MIASE – Detailed description of the MI

- Simulation parameter settings
  - time
    - start output time (time delay yes/no)
    - type of time used for the simulation
      - real time
      - cpu time
      - model initial time
      - model time
    - duration of simulation (consider different units)
    - number of intervals(or interval size)
  - simulation method used (KiSAO:0000005)
    - referencing the ontology
    - KiSAO:ID
    - termination criteria

# MIASE – Detailed description of the MI

- Plotting information
  - what has been plotted in the simulation
    - x-axis
    - y-axis
    - z-axis

```
<xs element name="plot">  
<xs:complexContent> <xs:sequence>  
  <xs:element name="x-Axis" type="xs:string" />  
  <xs:element name="y-Axis" type="xs:string" />  
  <xs:element name="z-Axis" type="xs:string"  
  use="optional" />  
</xs:sequence> </xs:complexContent>  
</xs:element>
```