

SBO

SBML

SBO

BioModels.net: semantics for model sharing

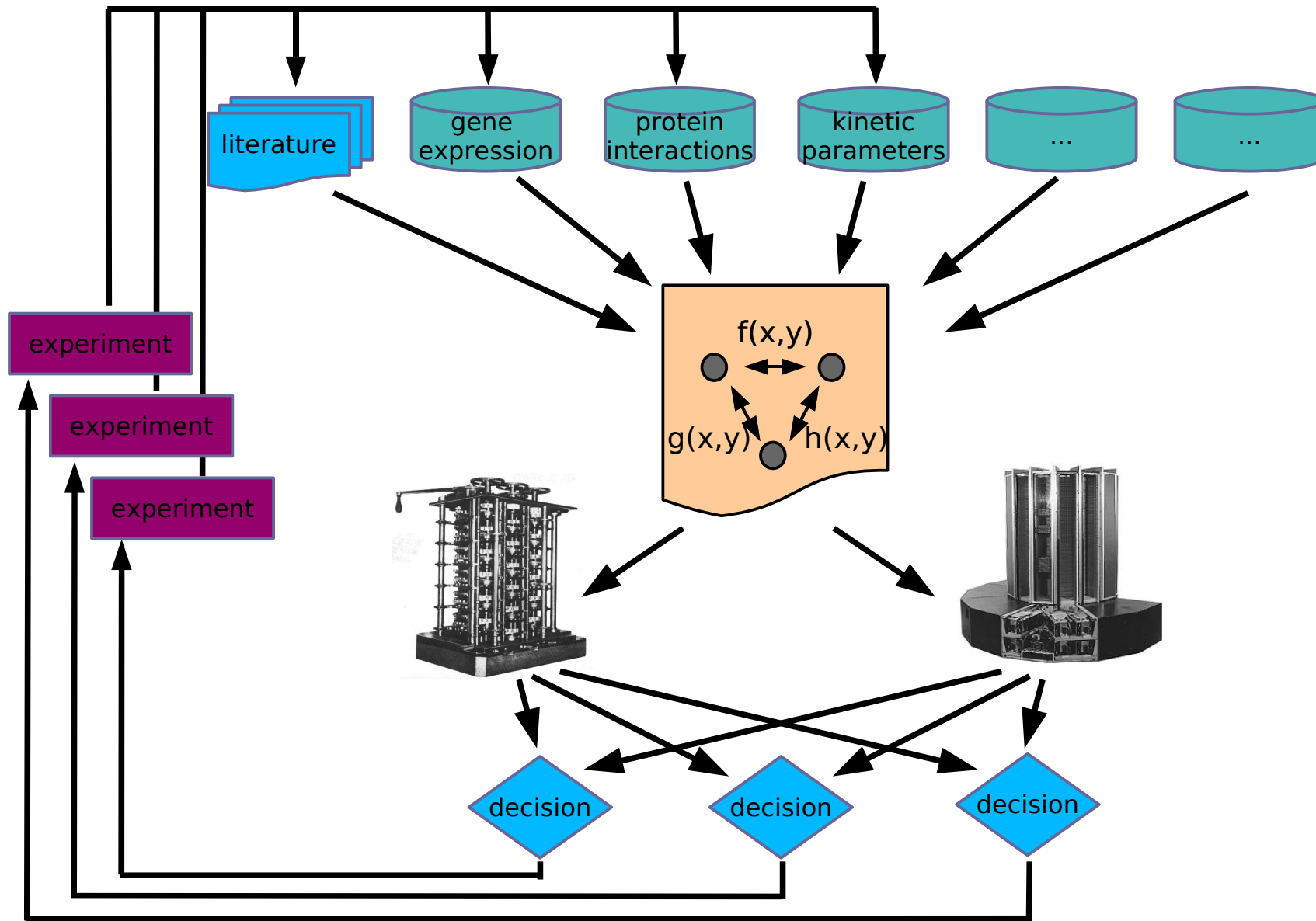
Nicolas Le Novère, EMBL-EBI, United-Kingdom

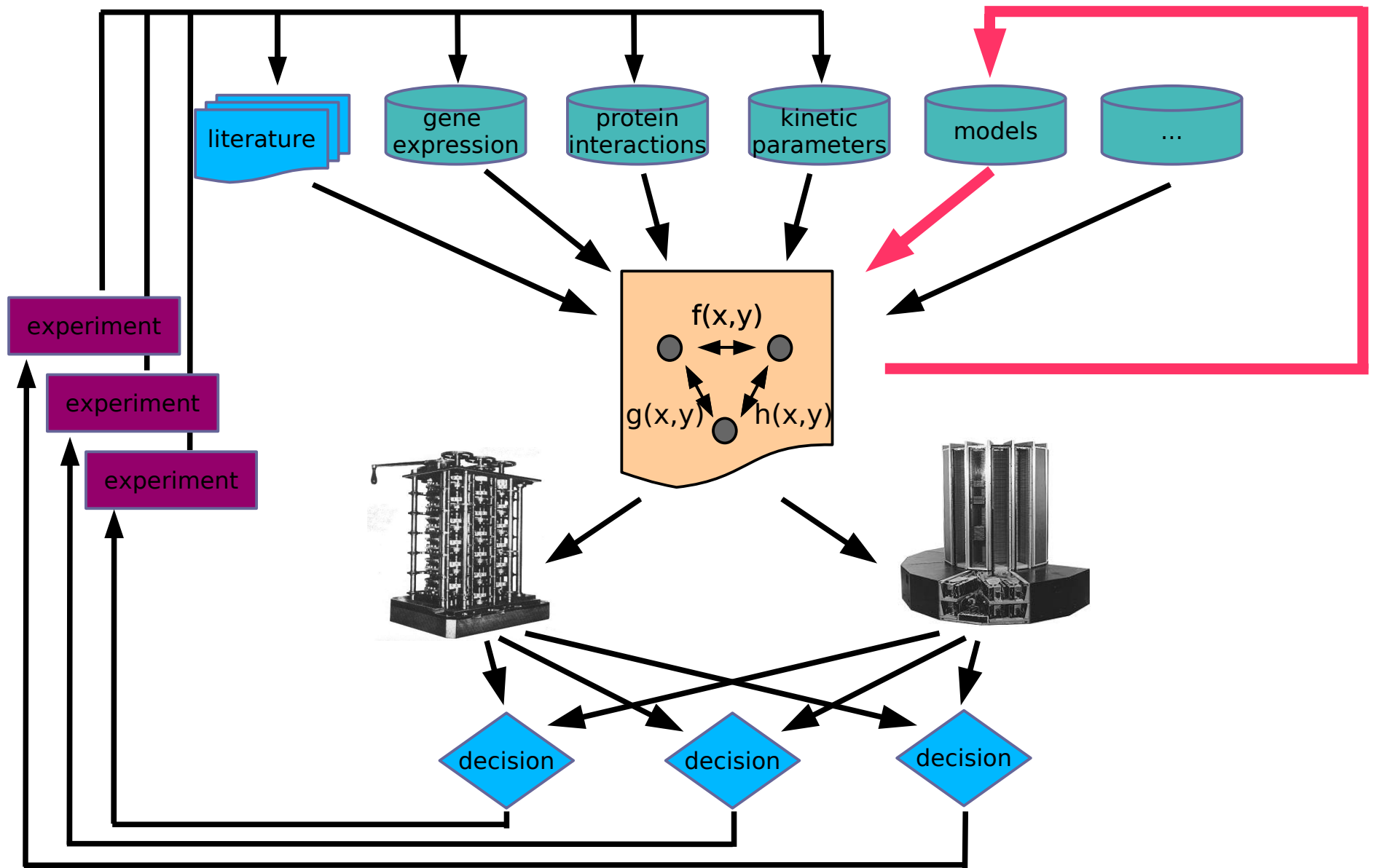
BioPAX

MIRIAM

SBGN



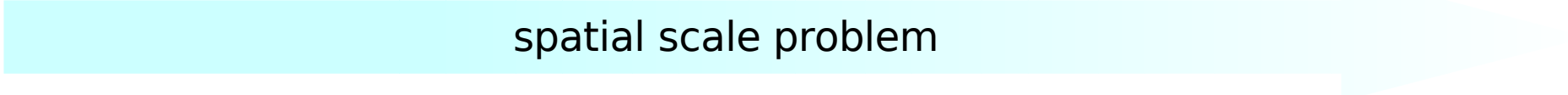
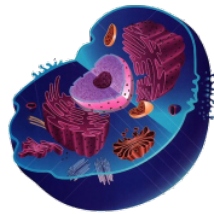
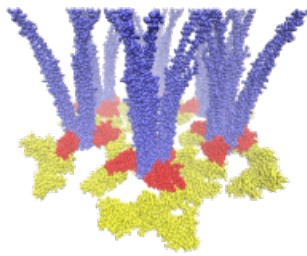
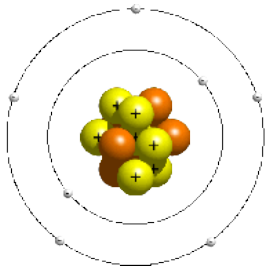


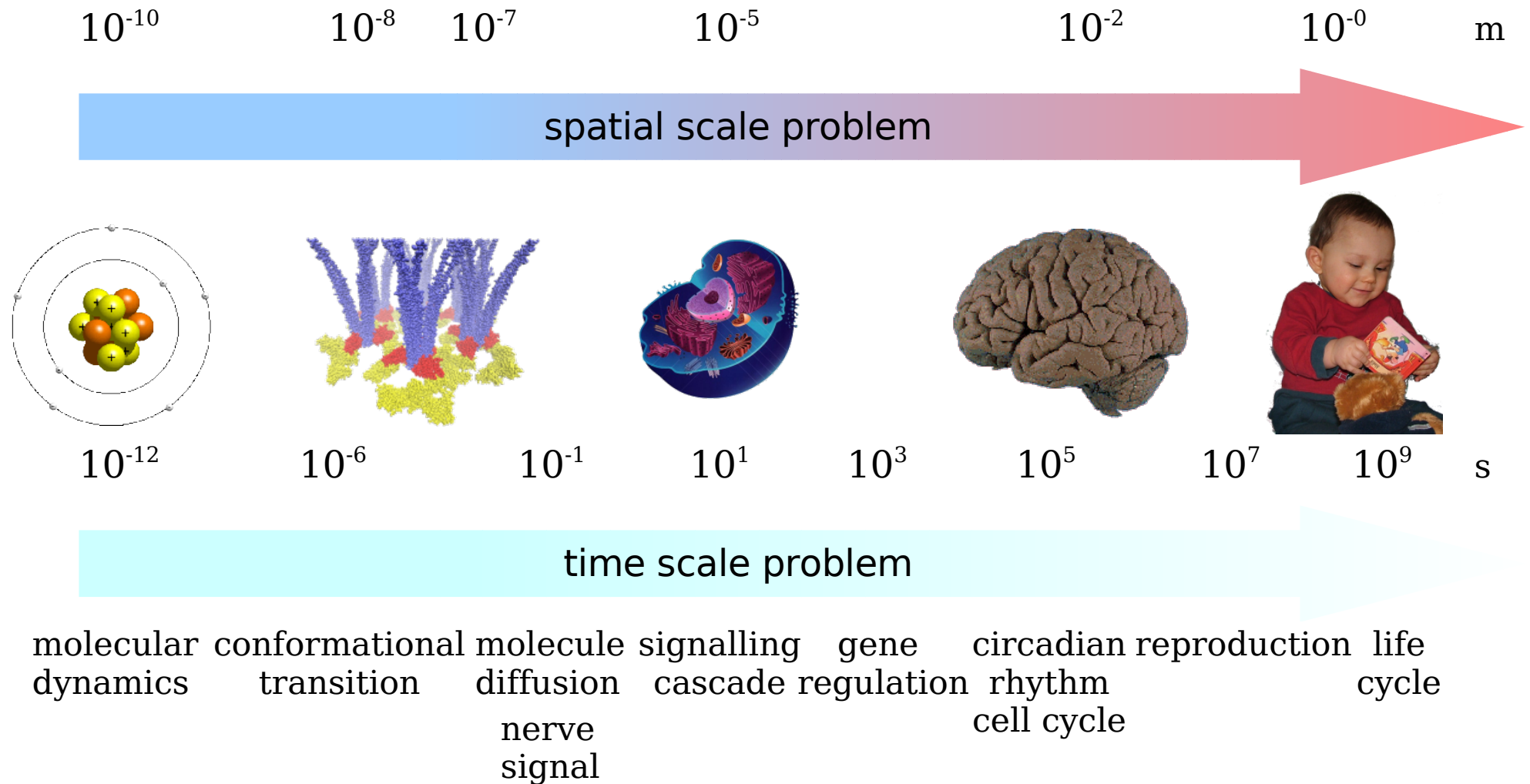


10^{-10}
 10^{-8}
 10^{-7}
 10^{-5}
 10^{-2}
 10^{-0}

m

spatial scale problem



- Molecular dynamics: to simulate $\propto 10^{-12}$ s requires $\propto 1$ s
- Particle diffusion: to simulate $\propto 10^{-6}$ s requires $\propto 1$ s
- Stochastic chemical kinetics: to simulate $\propto 1$ s requires $\propto 1$ s
- Continuous ODE: to simulate $\propto 10^3$ s requires $\propto 1$ s

$\Rightarrow$ Humongous stiffness: the speed of the whole simulation is determined by the quickest event



We need to reuse computational models

- The development of quantitative models of even simple living systems requires an extensive knowledge of biology, from biochemical reactions to physiology.



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- Very large pathways cannot be built in one shot. We are talking about hundreds of thousands of interactions ...

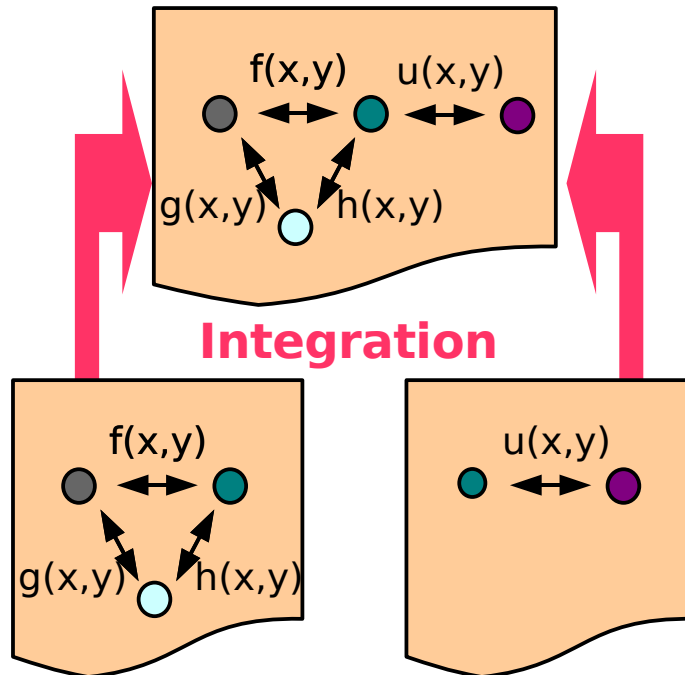


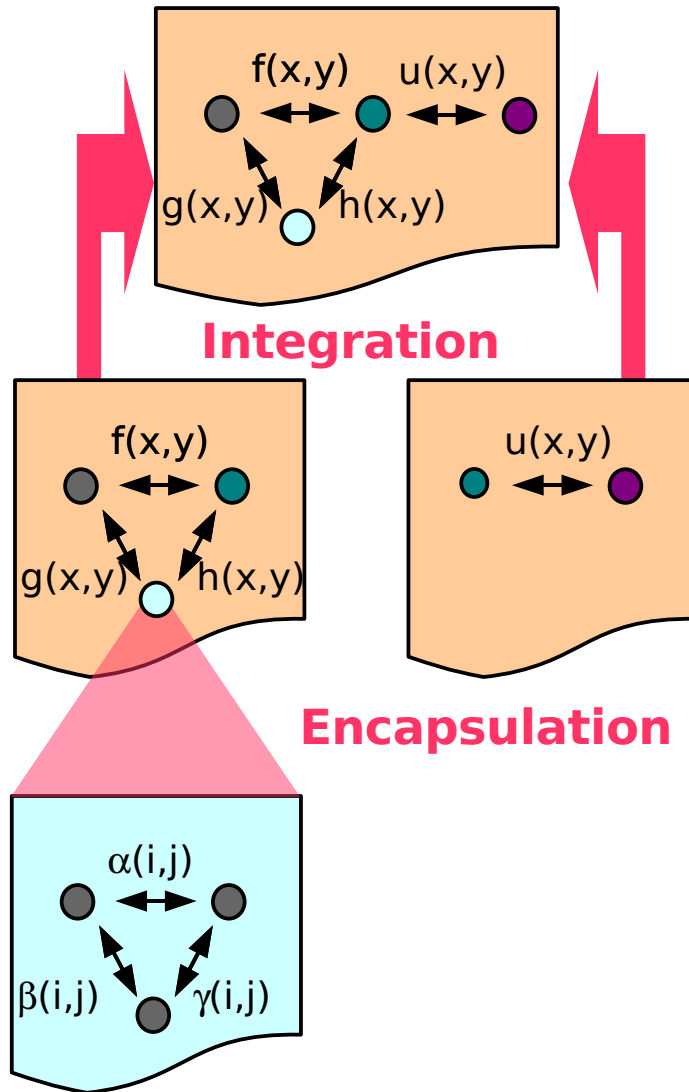
We need to reuse computational models

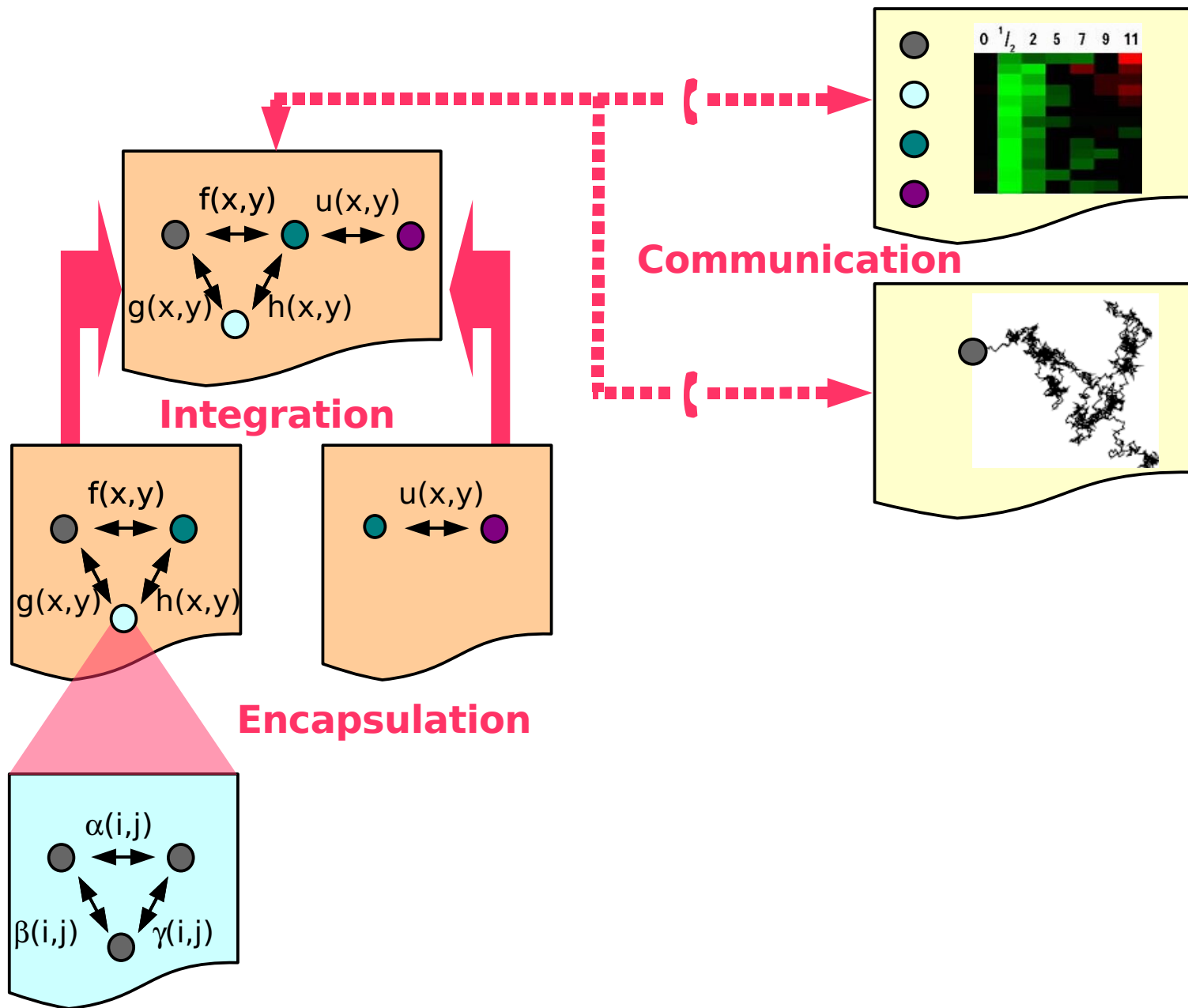
- The development of quantitative models of even simple living systems requires an extensive knowledge of biology, from biochemical reactions to physiology.
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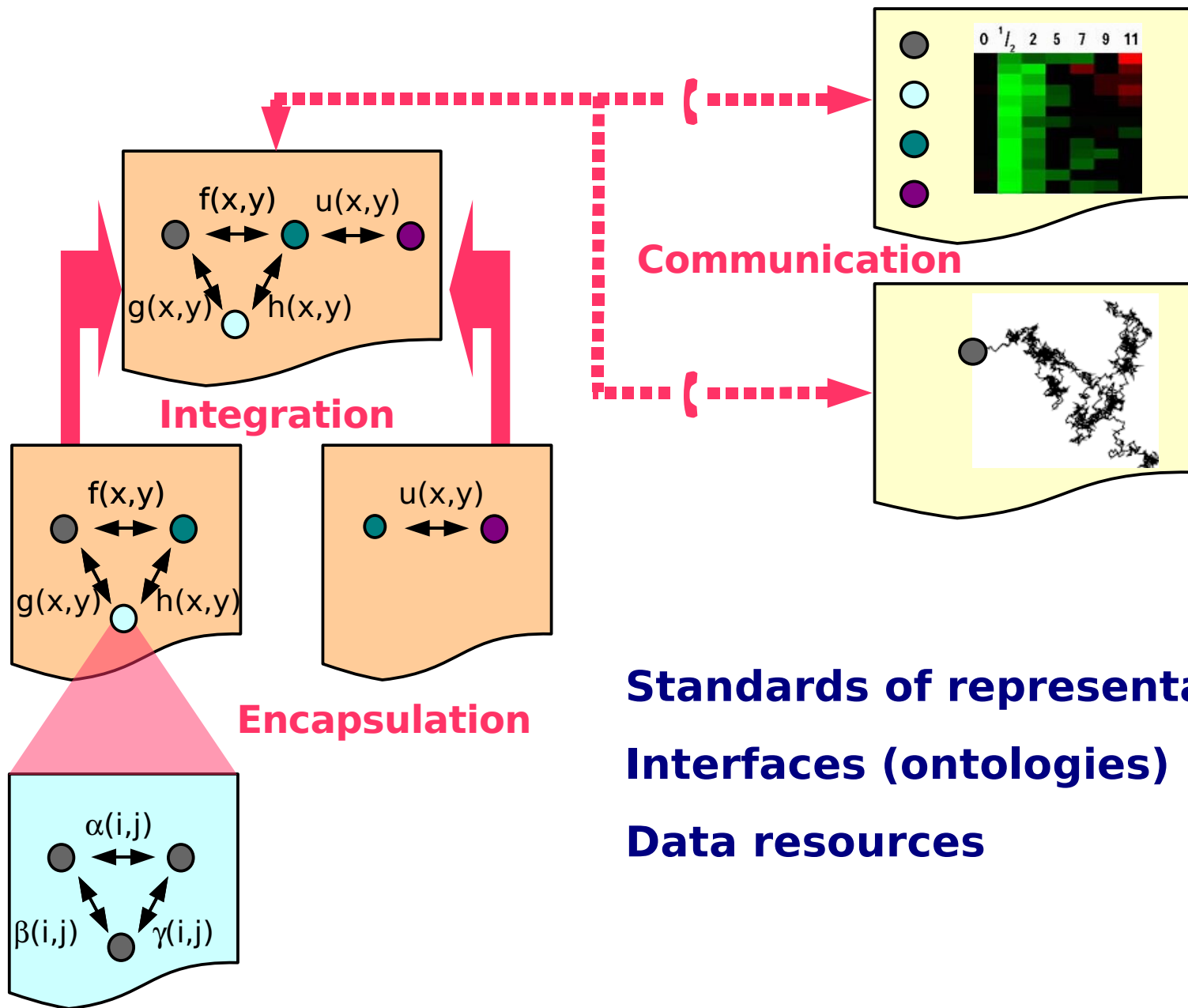
⇒ Nobody possesses the required knowledge. Moreover the time, money and energy necessary are prohibitive











“ The nice thing about standards is that there are so many to choose from”.
Attributed to Andrew S Tanenbaum





<http://www.cellml.org/>
Based on modules; scalable;



<http://www.neuroml.org/>
Flexible (expendable set of classes/schemas);



<http://brainml.org/>
Models are XML-schemas



<http://www.biopax.org/>
No kinetics; deep semantics; OWL



<http://www.sbgn.org/>
Graphical representation of interactions



<http://sbml.org/>
Rich kinetics; weak semantics; XML



The Systems Biology Markup Language (SBML) is a computer-readable format for representing **models of biochemical reaction networks**. SBML is applicable to metabolic networks, cell-signaling pathways, regulatory networks, and many others.

Internationally Supported and Widely Used

SBML has been evolving since mid-2000 through the efforts of an international group of software developers and users. Today, SBML is **supported by over 100 software systems**, including the following (where '*' indicates SBML support in development):

BALSA	Dizzy	Molecularizer	SBMLR
BASIS	E-CELL	Monod	SBMLSim
BIOCHAM	ecellJ	Narrator	SBMLToolbox
BioCharon	ESS	NetBuilder	SBLiD
ByoDyn	FluxAnalyzer	Oscill8	SBToolbox
BioCyc	Fluxor	PANTHER Pathway	SBW
BioGrid	Gepasi	PathArt	SClpath
BioModels	Gillespie2	PathScout	Sigmoid*
BioNetGen	HSMB	Pathway Analyser	SigPath
BioPathwise	HybridSBML	PathwayLab	SigTran
Bio Sketch Pad	INSILICO discovery	Pathway Tools	SIMBA
BioSens	JACOBIAN	PathwayBuilder	SimBiology
BioSPICE Dashboard	Jarnac	PATIKAwab	Simpathica
BioSpreadsheet	JDesigner	PaVESy	SimPheny*
BioTapestry	JigCell	PET	SimWiz
BioUML	JSim	PNK	SloppyCell
BSTLab	JWS Online	PottersWheel	SmartCell
CADLIVE	Karyote*	Reactome	SRS Pathway Editor
CellDesigner	KEGG2SBML	ProcessDB	StochSim
Cellerator	Kineticon	PROTON	StochKit
CellML2SBML	Kinsolver*	pysbml	STOCKS
Cellware	libSBML	PySCeS	TERANODE Suite
CL-SBML	MathSBML	runSBML	Trelis
CLEML	MesoRD	SABIO-RK	Virtual Cell
COPASI	MetaboLogica	SBML ODE Solver	WebCell
Cyto-Sim	MetaFluxNet	SBML-PET	WinSCAMP
Cytoscape	MMT2	SBMLEditor	XPPAUT
DBsolve	Modesto	SBMLmerge	

A Free and Open Language

Advances in biotechnology are leading to larger, more complex quantitative models. The systems biology

BioNetGen@VCell Release

(October 6, 2006) **BioNetGen@VCell** is a new release of BioNetGen, a tool for automatically generating a reaction network from user-specified rules for biomolecular interactions on the level of protein domains.

[read more](#)

PottersWheel supports SBML

(October 4, 2006) **PottersWheel 1.2 beta**, a MATLAB systems biology toolbox, supports model creation, fitting data, and designing new experiments.

[read more](#)

SBML Level 2 Version 2 Released!

(September 25, 2006) The final version of the **SBML Level 2 Version 2** specification is [now available!](#)

[read more](#)

SBML Wikipedia entry

(September 18, 2006) There is now an updated entry for SBML in Wikipedia. [Let us know](#) your suggestions for improvements.

[read more](#)

SBML Tutorial at ICSB 2006

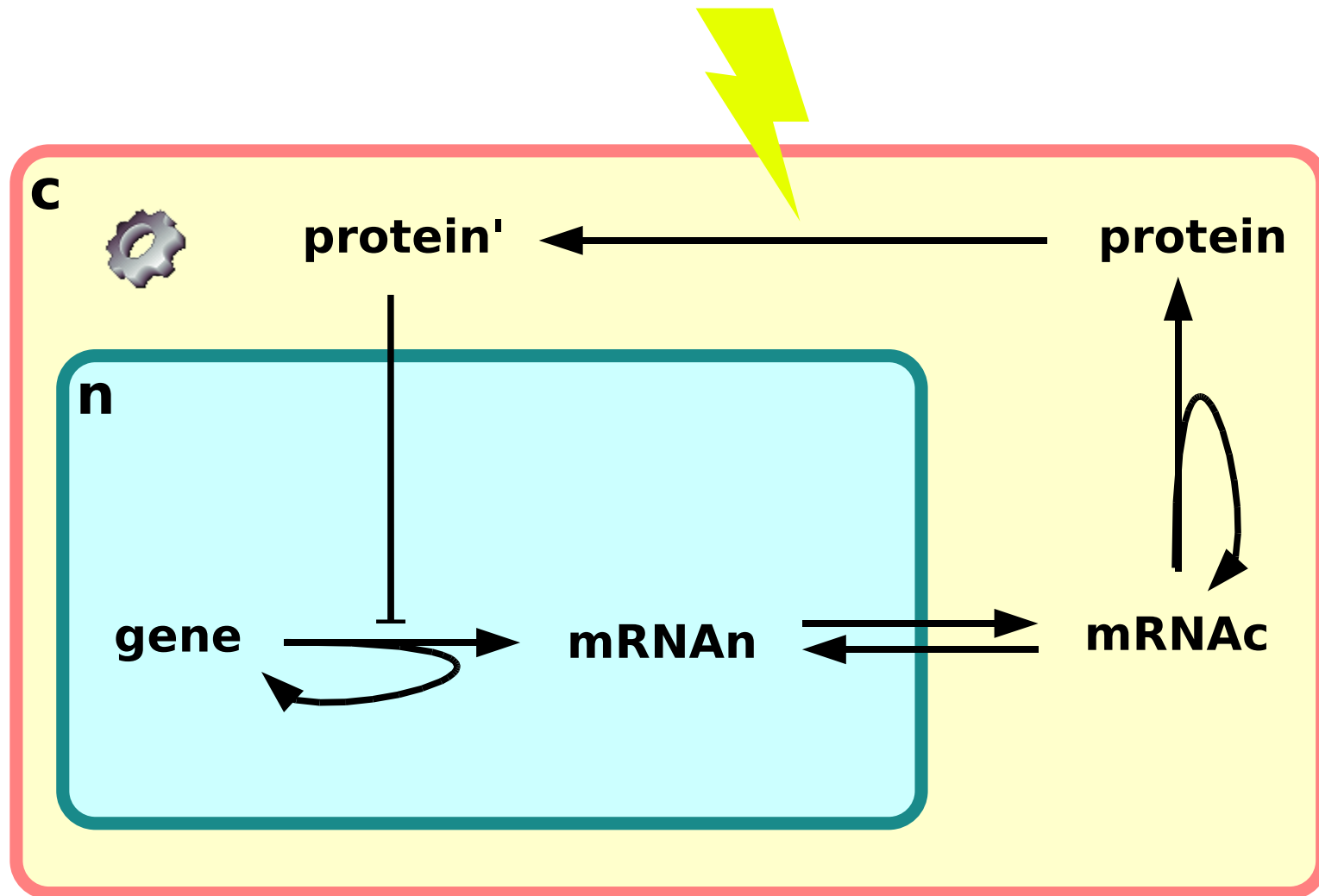
(September 8, 2006) Mike Hucka will be leading a tutorial on SBML this year at ICSB 2006 in Japan. The focus will be on the about-to-be-released SBML Level 2 Version 2.

[read more](#)

See [older news items](#).

"The goal of SBML is to help people to disagree as precisely as possible". Ed Franck, Argonne National Laboratory





```
<?xml version="1.0" encoding="UTF-8"?>
<sbml level="2" version="1" xmlns="http://www.sbml.org/sbml/level2">
  <model>
    <listOfCompartments>
      <compartment id="cell" />
    </listOfCompartments>
    <listOfSpecies>
      <species id="A" compartment="cell" initialConcentration="1"/>
      <species id="B" compartment="cell" initialConcentration="0"/>
    </listOfSpecies>
    <listOfParameters>
      <parameter id="kon" value="1"/>
    </listOfParameters>
    <listOfReactions>
      <reaction>
        <listOfReactants>
          <speciesReference species="A" />
        </listOfReactants>
        <listOfProducts>
          <speciesReference species="B" />
        </listOfProducts>
        <kineticLaw>
          <math xmlns="http://www.w3.org/1998/Math/MathML">
            <apply>
              <times />
              <ci>kon</ci>
              <ci>A</ci>
              <ci>cell</ci>
            </apply>
          </math>
        </kineticLaw>
      </reaction>
    </listOfReactions>
  </model>
</sbml>
```



- **Rate Rules** can describe the temporal evolution of any quantitative parameter, e.g. transmembrane voltage;
- **Events** can describe any discontinuous change, e.g. neurotransmitter release;
- A **species** is an entity participating to a reaction, **not always** a **chemical** entity:
 - It can be a molecule
 - It can be a cell
 - It can be an organ
 - It can be an organism

→ Remember, Systems Biology is scale-free!



- Level 1 (March 2001)
 - Predefined kinetics functions
 - Only one type of reactive substance
 - ISO646 encoding
- Level 2 (June 2003)
 - User-defined functions
 - Modifier species
 - Events
 - All math in MathML
 - Unicode encoding
 - IETF MIME-Type, see RFC3823
- Level 3 (?)

Hucka et al (2003)
Bioinformatics 19: 524-531

Hucka et al (2004)
IEE Systems Biology 1: 41-53



- Released on September 25th 2006
- Simpler and cleaner (units ...)
- Generic entities (compartmentType, speciesType)
→ path to generalised reactions
- Constraints and initialAssignments
- Controlled (MIRIAM) annotations (+ links to SBO)
- Backward compatible with Level 2 Version 1
- More detailed and bug-free specification ... 145 pages, 10pt, small margin.



- Modular SBML, with core + optional packages
- Graph Layout
- Generalised reactions (probable)
- Model composition (probable)
- Complex species (probable)
- Arrays or sets (maybe)
- Geometry (maybe)
- Movements (maybe)
- Dynamic compartments (maybe)
- ???



- An SBML model lists physical entities, but does not identify them properly.
- An SBML model contains mathematical expressions, but does not tell-us what they characterise and how.
- An SBML constructed for a certain modelling approach cannot be used straight-away within another modelling framework.

⇒ SBML models cannot be easily searched
SBML models cannot be easily converted
SBML models cannot be easily merged



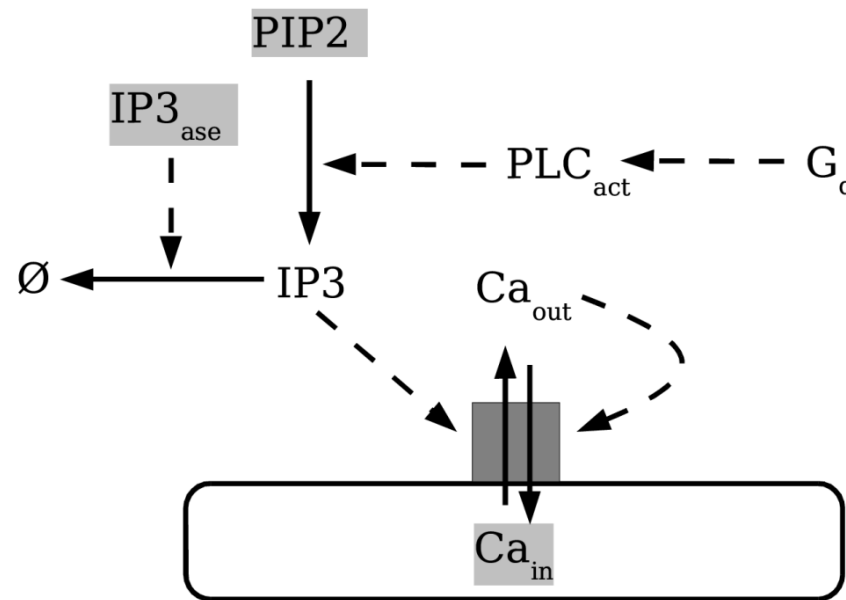
Minimum Information Requested In the Annotation of biochemical Models

Le Novère N., Finney A., Hucka M., Bhalla U., Campagne F., Collado-Vides J.,
Crampin E., Halstead M., Klipp E., Mendes P., Nielsen P., Sauro H., Shapiro B.,
Snoep J.L., Spence H.D., Wanner B.L.
Nature Biotechnology (2005), 23: 1509-1515

<http://www.ebi.ac.uk/compneur-srv/miriam/>

- The model must be encoded in a public, standardized, machine-readable format (SBML, CellML, GENESIS ...)
- The model must comply with the standard in which it is encoded!
- The model must be clearly related to a single reference description. If a model is composed from different parts, there should still be a description of the derived/combined model.
- The encoded model structure must reflect the biological processes listed in the reference description.
- The model must be instantiated in a simulation: All quantitative attributes have to be defined, including initial conditions.
- When instantiated, the model must be able to reproduce all results given in the reference description within an epsilon (algorithms, round-up errors)





$$k_1 = k_2 = k_3 = 1 \text{ s}^{-1}$$

$$Km_1 = 10^{-7} \text{ M}, Km_2 = 10^{-8}, Km_3 = 2.10^{-6} \text{ M}$$

$$K_A = 10^{-11}, m = 4, n = 3, \alpha = 0.001$$

$$[Ca_{in}] = [IP3R] = [PLC_{tot}] = [PIP2] = [IP3_{ase}] = 0.001 \text{ M}$$

$$[G_q] = 0.01 \text{ M}, [Ca_{out}] = [IP3] = [PLC_{act}] = 0 \text{ M}$$

$$\frac{d[Ca_{out}]}{dt} = \frac{k_1[IP3R] * ([Ca_{in}] - [Ca_{out}])}{Km_1 + |[Ca_{in}] - [Ca_{out}]|} * \frac{[IP3]^m}{K_A + [IP3]^m}$$

$$\frac{d[IP3]}{dt} = \frac{k_2[PLC_{act}] * [PIP2]}{Km_2 + [PIP2]} - \frac{k_3[IP3_{ase}] * [IP3]}{Km_3 + [IP3]}$$

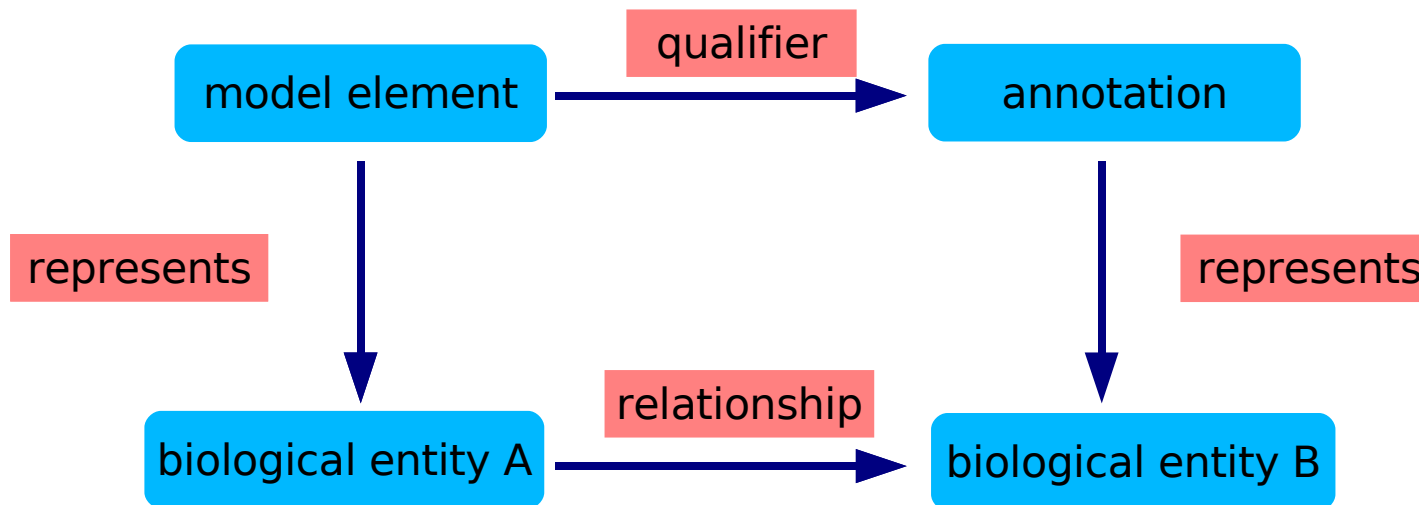
$$\frac{d[PLC_{act}]}{dt} = \frac{[G_q]^n}{\alpha + [G_q]^n} * [PLC_{tot}]$$



- The model has to be named.
- A citation of the reference description must be joined (complete citation, unique identifier, unambiguous URL). The citation should permit to identify the *authors* of the model.
- The name and contact of model *creators* must be joined.
- The date and time of creation and last modification should be specified. An history is useful but not required.
- The model should be linked to a precise statement about the terms of distribution. MIRIAM does not require “freedom of use” or “no cost”.



- The annotation must permit to unambiguously relate a piece of knowledge to a model constituent.
- The referenced information should be described using a triplet {data-type, identifier, qualifier}



- The community has to agree on a set of standard valid data-types. A database and the associated API (WebServices) have been developed at the EBI to provide the generation and interpretation of URIs.



creators	Joe User (juser@eden.com), Anne Other (aother@eden.com)			
creation date	01 January 0000			
last modification	31 May 2005			
Constituent	Data Type	Identifier	Qualifier	Meaning
model	http://www.pubmed.gov/	0000000		
	http://www.taxonomy.org/	9606		<i>Homo sapiens</i>
	http://www.geneontology.org/	GO:0007204	IsVersionOf	<i>positive regulation of cytosolic ca2+ concentration</i>
	http://www.geneontology.org/	GO:0051279	IsVersionOf	<i>regulation of release of sequestered ca2+ into cytop</i>
	http://www.genome.jp/kegg/pathway	hsa04020	IsPartOf	<i>Calcium signaling pathway—H sapiens</i>
	http://www.genome.jp/kegg/pathway	hsa04070	IsPartOf	<i>Phosphatidylinositol signaling system—H sapiens</i>
compartment ER	http://www.geneontology.org/	GO:0005790		<i>smooth endoplasmic reticulum</i>
reactant Ca _{in}	http://www.ebi.ac.uk/chebi/	CHEBI:29108		<i>calcium(2+)</i>
compartment cytoplasm	http://www.geneontology.org/	GO:0005737		<i>cytoplasm</i>
reactant Ca _{out}	http://www.ebi.ac.uk/chebi/	CHEBI:29108		<i>calcium(2+)</i>
reactant IP3	http://www.ebi.ac.uk/chebi/	CHEBI:16595		<i>1D-myo-inositol 1,4,5-tris(dihydrogen phosphate)</i>
reactant PIP2	http://www.ebi.ac.uk/chebi/	CHEBI:18348		<i>1-phosphatidyl-1D-myo-inositol 4,5-bisphosphate</i>
reactant IP3R	http://www.uniprot.org/	Q14643	HasVersion	<i>Inositol 1,4,5-trisphosphate receptor type 1</i>
	http://www.uniprot.org/	Q14571	HasVersion	<i>Inositol 1,4,5-trisphosphate receptor type 2</i>
	http://www.uniprot.org/	Q14573	HasVersion	<i>Inositol 1,4,5-trisphosphate receptor type 3</i>
reactant PLC _{act}	http://www.uniprot.org/	Q9NQ66	IsVersionOf	<i>PIP2 phosphodiesterase β1</i>
reactant PLC _{tot}	http://www.uniprot.org/	Q9NQ66		<i>PIP2 phosphodiesterase β1</i>
reactant IP3 _{ase}	http://www.uniprot.org/	Q14642		<i>Type I inositol-1,4,5-trisphosphate 5-phosphatase</i>
reactant G _q	http://www.uniprot.org/	Q6NT27		<i>Guanine nucleotide binding protein Gq</i>
reaction Ca _{release}	http://www.geneontology.org/	GO:0005220		<i>IP3-sensitive calcium-release channel activity</i>
	http://www.geneontology.org/	GO:0008095	IsVersionOf	<i>IP3 receptor activity</i>
reaction IP3 _{production}	http://www.geneontology.org/	GO:0004435	IsVersionOf	<i>phosphoinositide phospholipase C activity</i>
	http://www.ec-code.org/	3.1.4.11	IsVersionOf	<i>phosphoinositide phospholipase C</i>
reaction IP3 _{degradation}	http://www.ec-code.org/	3.1.3.56	IsVersionOf	<i>inositol-polyphosphate 5-phosphatase</i>
reaction PLC _{activation}	http://www.geneontology.org/	GO:0007200		<i>G-protein signaling coupled to IP3 2nd messenger</i>

```
<species metaid="metaid_0000055"
  id="boundEGFReceptor"
  compartment="cell"
  initialConcentration="0">
  <annotation>
    <rdf:RDF xmlns:rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns#"
      xmlns:bqbiol="http://biomodels.net/biology-qualifiers/"
      xmlns:bqmodel="http://biomodels.net/model-qualifiers/">
      <rdf:Description rdf:about="#metaid_0000055">
        <bqbiol:hasPart>
          <rdf:Bag>
            <rdf:li rdf:resource="http://www.uniprot.org/#Q9QX70"/>
            <rdf:li rdf:resource="http://www.uniprot.org/#P07522"/>
          </rdf:Bag>
        </bqbiol:hasPart>
      </rdf:Description>
    </rdf:RDF>
  </annotation>
</species>
```



Browse data-types

Brief overview of the different data-types stored in *MIRIAM*.

Name	URI	Definition
BIND	http://www.bind.ca/	BIND is a database of protein-protein interactions. This data-resource is not open-access.
ChEBI	http://www.ebi.ac.uk/chebi/	Chemical Entities of Biological Interest (ChEBI) is a freely available dictionary of molecular entities focused on 'small' chemical compounds.
Ensembl	http://www.ensembl.org/	Ensembl is a joint project between EMBL - EBI and the Sanger Institute to develop a software system which produces and maintains automatic annotation on selected eukaryotic genomes.
Enzyme Nomenclature	http://www.ec-code.org/	The Enzyme Classification contains the recommendations of the Nomenclature Committee of the International Union of Biochemistry and Molecular Biology on the nomenclature and classification of enzyme-catalysed reactions.
UniProt	http://www.uniprot.org/	UniProt (Universal Protein Resource) is the world's most comprehensive catalog of information on proteins. It is a central repository of protein sequence and function created by joining the information contained in Swiss-Prot, TrEMBL, and PIR.
Taxonomy	http://www.taxonomy.org/	The taxonomy contains the relationships between all living forms for which nucleic acid or protein sequence have been determined.
DOI	http://www.doi.org/	The Digital Object Identifier System is for identifying content objects in the digital environment.
Gene Ontology	http://www.geneontology.org/	The Gene Ontology project provides a controlled vocabulary to describe gene and gene product attributes in any organism.
ICD	http://www.who.int/classifications/icd/	The International Classification of Diseases is the international standard diagnostic classification for all general epidemiological and many health management purposes.
IntAct	http://www.ebi.ac.uk/intact/	IntAct provides a freely available, open source database system and analysis tools for protein interaction data.
InterPro	http://www.ebi.ac.uk/interpro/	InterPro is a database of protein families, domains and functional sites in which identifiable features found in known proteins can be applied to unknown protein sequences.
KEGG Pathway	http://www.genome.jp/kegg/pathway/	KEGG PATHWAY is a collection of manually drawn pathway maps representing our knowledge on the molecular interaction and reaction networks.
KEGG Compound	http://www.genome.jp/kegg/compound/	KEGG compound contains our knowledge on the universe of chemical substances that are relevant to life.
KEGG Reaction	http://www.genome.jp/kegg/reaction/	KEGG reaction contains our knowledge on the universe of reactions that are relevant to life.
PubMed	http://www.pubmed.gov/	PubMed is a service of the U.S. National Library of Medicine that includes citations from MEDLINE and other life science journals for biomedical articles back to the 1950s.
OMIM	http://www.ncbi.nlm.nih.gov/OMIM/	Online Mendelian Inheritance in Man is a catalog of human genes and genetic disorders.



- Browse
- Request
- Submission
- XML Export
- Sign In

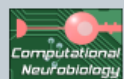
- News
- Web Services
- BioModels
- Qualifiers
- FAQ
- Contact





- Browse
- Request
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- XML Export
- Sign In

- News
- Web Services
- BioModels
- Qualifiers
- FAQ
- Contact



Data-type Enzyme Nomenclature

<u>Name</u>	
Official	Enzyme Nomenclature
Synonyms	Enzyme Classification
	EC code
	EC
<u>URIs</u>	
Official URL	http://www.ec-code.org/
Official URN	urn:lsid:ec-code.org
Deprecated	http://www.ebi.ac.uk/IntEnz/
<u>Information</u>	
Definition	The Enzyme Classification contains the recommendations of the Nomenclature Committee of the International Union of Biochemistry and Molecular Biology on the nomenclature and classification of enzyme-catalysed reactions.
Identifier Pattern	<code>^d+ d+\.(- d+) d+\.d+\.(- d+) d+\.d+\.d+\.(- d+)\$</code>
<u>Physical Locations</u>	
Resource #1	Data Entry http://www.ebi.ac.uk/intenz/query?cmd=SearchEC&ec=\$id
	Data Resource http://www.ebi.ac.uk/intenz/
Resource #2	Data Entry http://www.genome.jp/dbget-bin/www_bget?ec:\$id
	Data Resource http://www.genome.jp/dbget-bin/www_bfind?enzyme
Resource #3	Data Entry http://us.expasy.org/cgi-bin/nicezyme.pl?\$id
	Data Resource http://us.expasy.org/enzyme/
<u>Documentation</u>	
URL(s)	http://www.chem.qmul.ac.uk/iubmb/enzyme/
	http://www.ncbi.nlm.nih.gov/entrez/query.fcgi?cmd=Retrieve&db=pubmed&dopt=Abstract&list_uids=10812475
	http://srs.ebi.ac.uk/srsbin/cgi-bin/wgetz?-view+MedlineFull+[medline-PMID:10812475]

[Go back](#)

[Top](#)

Last modification: Wed Nov 15 2006

[Contact](#)

creators Joe User (juser@eden.com), Anne Other (aother@eden.com)
creation date 01 January 0000
last modification 31 May 2005

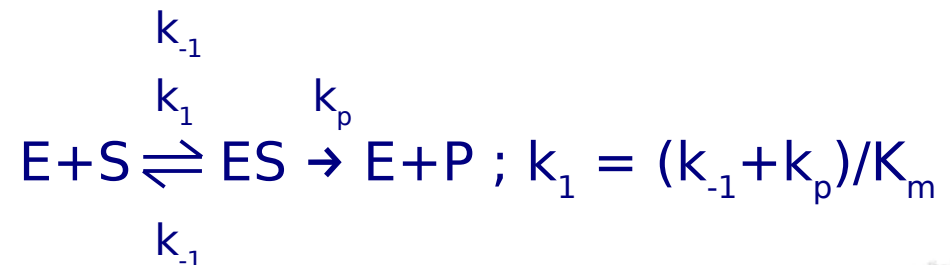
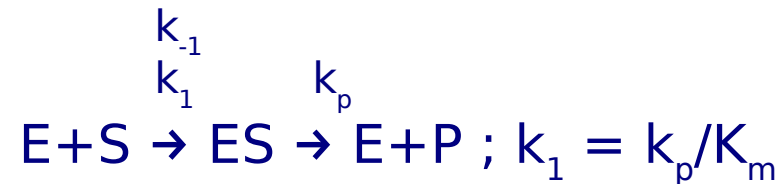
What is common?

Constituent	Data Type	Identifier	Qualifier	Meaning
model	http://www.pubmed.gov/ http://www.taxonomy.org/ http://www.geneontology.org/ http://www.geneontology.org/ http://www.genome.jp/kegg/pathway http://www.genome.jp/kegg/pathway	0000000 9606 GO:0007204 GO:0051279 hsa04020 hsa04070	 IsVersionOf IsVersionOf IsPartOf IsPartOf	 <i>Homo sapiens</i> <i>positive regulation of cytosolic ca2+ concentration</i> <i>regulation of release of sequestered ca2+ into cytop</i> <i>Calcium signaling pathway—H sapiens</i> <i>Phosphatidylinositol signaling system—H sapiens</i>
compartment ER	http://www.geneontology.org/	GO:0005790		<i>smooth endoplasmic reticulum</i>
reactant Ca _{in}	http://www.ebi.ac.uk/chebi/	CHEBI:29108		<i>calcium(2+)</i>
compartment cytoplasm	http://www.geneontology.org/	GO:0005737		<i>cytoplasm</i>
reactant Ca _{out}	http://www.ebi.ac.uk/chebi/	CHEBI:29108		<i>calcium(2+)</i>
reactant IP3	http://www.ebi.ac.uk/chebi/	CHEBI:16595		<i>1D-myo-inositol 1,4,5-tris(dihydrogen phosphate)</i>
reactant PIP2	http://www.ebi.ac.uk/chebi/	CHEBI:18348		<i>1-phosphatidyl-1D-myo-inositol 4,5-bisphosphate</i>
reactant IP3R	http://www.uniprot.org/ http://www.uniprot.org/ http://www.uniprot.org/	Q14643 Q14571 Q14573	HasVersion HasVersion HasVersion	<i>Inositol 1,4,5-trisphosphate receptor type 1</i> <i>Inositol 1,4,5-trisphosphate receptor type 2</i> <i>Inositol 1,4,5-trisphosphate receptor type 3</i>
reactant PLC _{act}	http://www.uniprot.org/	Q9NQ66	IsVersionOf	<i>PIP2 phosphodiesterase β1</i>
reactant PLC _{tot}	http://www.uniprot.org/	Q9NQ66		<i>PIP2 phosphodiesterase β1</i>
reactant IP3 _{ase}	http://www.uniprot.org/	Q14642		<i>Type I inositol-1,4,5-trisphosphate 5-phosphatase</i>
reactant G _q	http://www.uniprot.org/	Q6NT27		<i>Guanine nucleotide binding protein Gq</i>
reaction Ca _{release}	http://www.geneontology.org/ http://www.geneontology.org/	GO:0005220 GO:0008095	 IsVersionOf	<i>IP3-sensitive calcium-release channel activity</i> <i>IP3 receptor activity</i>
reaction IP3 _{production}	http://www.geneontology.org/ http://www.ec-code.org/	GO:0004435 3.1.4.11	IsVersionOf IsVersionOf	<i>phosphoinositide phospholipase C activity</i> <i>phosphoinositide phospholipase C</i>
reaction IP3 _{degradation}	http://www.ec-code.org/	3.1.3.56	IsVersionOf	<i>inositol-polyphosphate 5-phosphatase</i>
reaction PLC _{activation}	http://www.geneontology.org/	GO:0007200		<i>G-protein signaling coupled to IP3 2nd messenger</i>

```
<reaction>
  <listOfReactants>
    <speciesReference species="S" />
  </listOfReactants>
  <listOfProducts>
    <speciesReference species="P" />
  </listOfProducts>
  <listOfModifiers>
    <speciesReference species="E" />
  </listOfModifiers>
  <kineticLaw>
    <listOfParameters>
      <parameter id="Km"/>
      <parameter id="kp"/>
    </listOfParameters>
    <math xmlns="http://www.w3.org/1998/Math/MathML">
      <apply>
        <divide/><apply>
          <times/><ci>E</ci>
          <ci>kp</ci>
          <ci>S</ci>
        </apply>
        <apply>
          <plus/><ci>Km</ci>
          <ci>S</ci>
        </apply>
      </apply>
    </math>
  </kineticLaw>
</reaction>
```



Import in a discrete simulator



The Systems Biology Ontology

SBO

<http://www.ebi.ac.uk/sbo/>

- Ontology: A set of elements of knowledge linked with sense-bearing relationships.
- Each term of an ontology is associated to a perennial identifier. Once created a term is never destroyed. It can be merged with another, or made obsolete, but it still exists.
- An ontology is an evolving structure: It can cope with an increase or refinement of knowledge. No need to reconstruct everything as with the taxonomies.
- An ontology is a Direct Acyclic Graph, and not a hierarchy. A term can possess more than one parent.
- Ontologies are stored in standard machine-readable formats. They can be subjected to automatic treatments.



- Types and roles of reaction participants, including terms like “substrate”, “catalyst” etc., but also “macromolecule”, or “channel”.
- Parameter used in quantitative models. This vocabulary includes terms like “Michaelis constant”, “forward unimolecular rate constant” etc.
- Mathematical expressions. Examples of terms are “mass action kinetics”, “Henri-Michaelis-Menten equation” etc. Each term contains a precise mathematical expression stored as a MathML lambda function. The variables refer to the CVs described above.
- Modelling framework to precise how to interpret the rate-law. E.g. “continuous modelling”, “discrete modelling” etc.
- Event type, such as “catalysis” or “addition of a chemical group”.



SBO Ontology Browser

SBO::Systems Biology Ontology

[Refresh tree](#)

sbo

- quantitative parameter
- modelling framework
- mathematical expression
 - rate law
 - mass action kinetics
 - Hill equation
 - enzyme kinetics
 - kinetics of non-modulated non-interacting enzymes
 - kinetics of unireactant enzymes
 - kinetics of non-modulated unireactant enzymes
 - Henri-Michaelis Menten equation
 - Van Slyke-Cullen equation
 - Briggs-Haldane equation
 - normalised kinetics of unireactant enzymes
 - simple uncompetitive inhibition of unireactant enzymes
 - competitive inhibition of unireactant enzymes
 - competitive inhibition of unireactant enzymes
 - mixed-type inhibition by mutually exclusive binding
 - obsolete mathematical expression
- event
- participant type

 "is a" relationship
 "part-of" relationship

[Top](#)

http://www.ebi.ac.uk - SBO::Systems Biology Ontology - Mozilla

SBO:0000031 Briggs-Haldane equation

Definition

Rate-law presented in "G.E. Briggs and J.B.S. Haldane (1925) A note on the kinetics of enzyme action, Biochem. J., 19: 339-339". It is a general rate equation that does not require the restriction of equilibrium of Henri-Michaelis-Menten or irreversible reactions of Van Slyke, but instead make the hypothesis that the complex enzyme-substrate is in quasi-steady-state. Although of the same form than the Henri-Michaelis-Menten equation, it is semantically different since Km now represents a pseudo-equilibrium constant, and is equal to the ratio between the rate of consumption of the complex (sum of dissociation of substrate and generation of product) and the association rate of the enzyme and the substrate.

MathML

$$\text{<math xmlns='http://www.w3.org/1998/Math/MathML'>}$$
$$\text{<semantics definitionURL='http://biomodels.net/SBO/#SBO:0000062'>}$$
$$\text{<math>}$$
$$\text{<bvar><ci definitionURL='http://biomodels.net/SBO/#SBO:0000025'>kcat</ci></bvar>}$$
$$\text{<bvar><ci definitionURL='http://biomodels.net/SBO/#SBO:0000015'>S</ci></bvar>}$$
$$\text{<bvar><ci definitionURL='http://biomodels.net/SBO/#SBO:0000027'>Km</ci></bvar>}$$
$$\text{<math>}$$
$$\text{</semantics>}$$
$$\text{</math>}$$

Comment

Parent(s)

SBO:0000028 kinetics of non-modulated unireactant enzymes (is a)

Children

Done


```
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    <speciesReference species="A" sboTerm="SBO:0000015"/>
  </listOfReactants>
  <listOfProducts>
    <speciesReference species="B" sboTerm="SBO:0000011"/>
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  </listOfModifiers>
  <kineticLaw sboTerm="SBO:0000031">
    <listOfParameters>
      <parameter id="U" sboTerm="SBO:0000008"/>
      <parameter id="V" sboTerm="SBO:0000025"/>
    </listOfParameters>
  </kineticLaw>
</reaction>
```

continuous simulator

$$v = [C] \times V \times \frac{[A]}{(U + [A])}$$

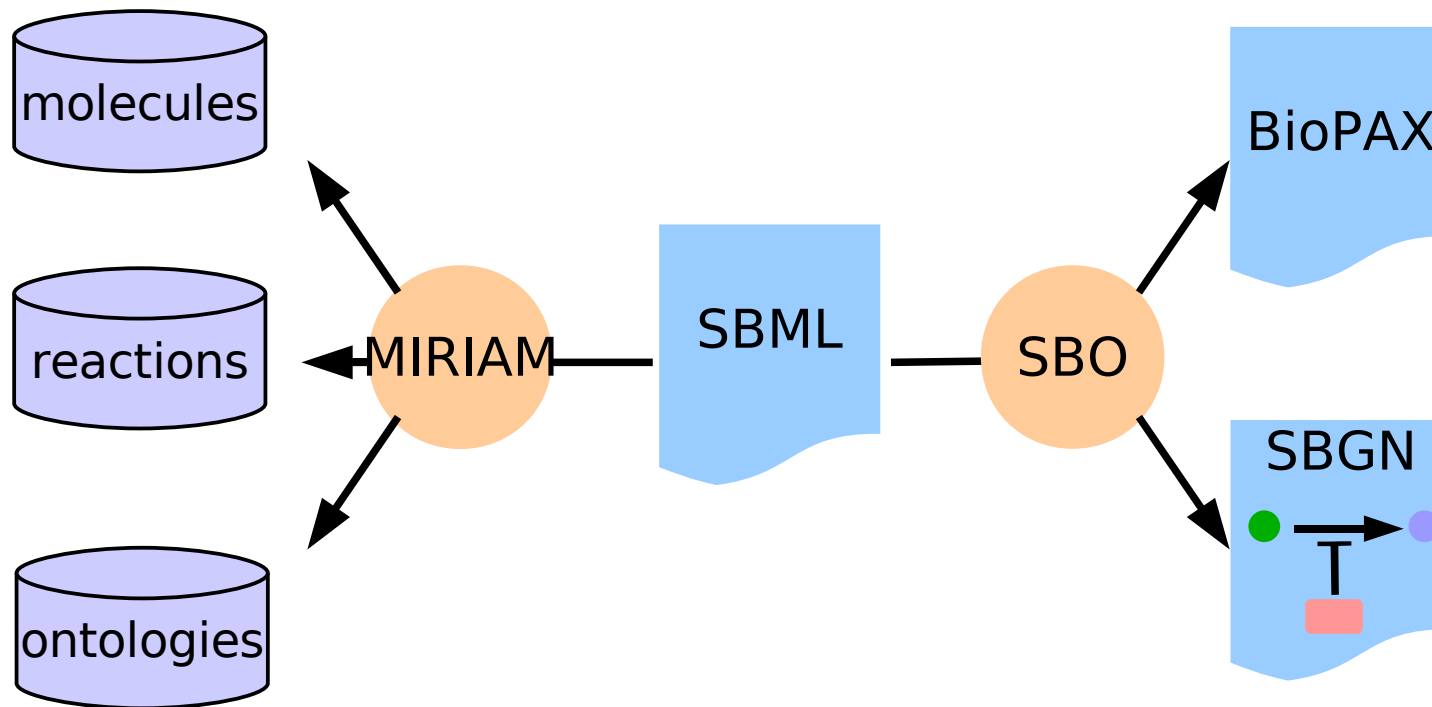
discrete simulator

$$v1 = \frac{(k_{-1} + V)}{U} * [A] * [C]$$

$$v2 = k_{-1} * [D]$$

$$v3 = V * [D]$$





- Neither focussed on a particular biological substrate or process, nor specialised on a given modelling approach
- Real “searchable” database rather than mere repository
- Models thoroughly verified, structure and results, and annotated
- International collaboration rather than a one-group effort
- Freely available and reusable
- Long-term commitment and secure funding



BioModels Database: A Free, Centralized Database of Curated, Published, Quantitative Kinetic Models of Biochemical and Cellular Systems

Le Novère N., Bornstein B., Broicher A., Courtot M., Donizelli M., Dharuri H., Li
L., Sauro H., Schilstra M., Shapiro B., Snoep J.L., Hucka M.
Nucleic Acids Research, (2006), 34: D689-D691

BioModels

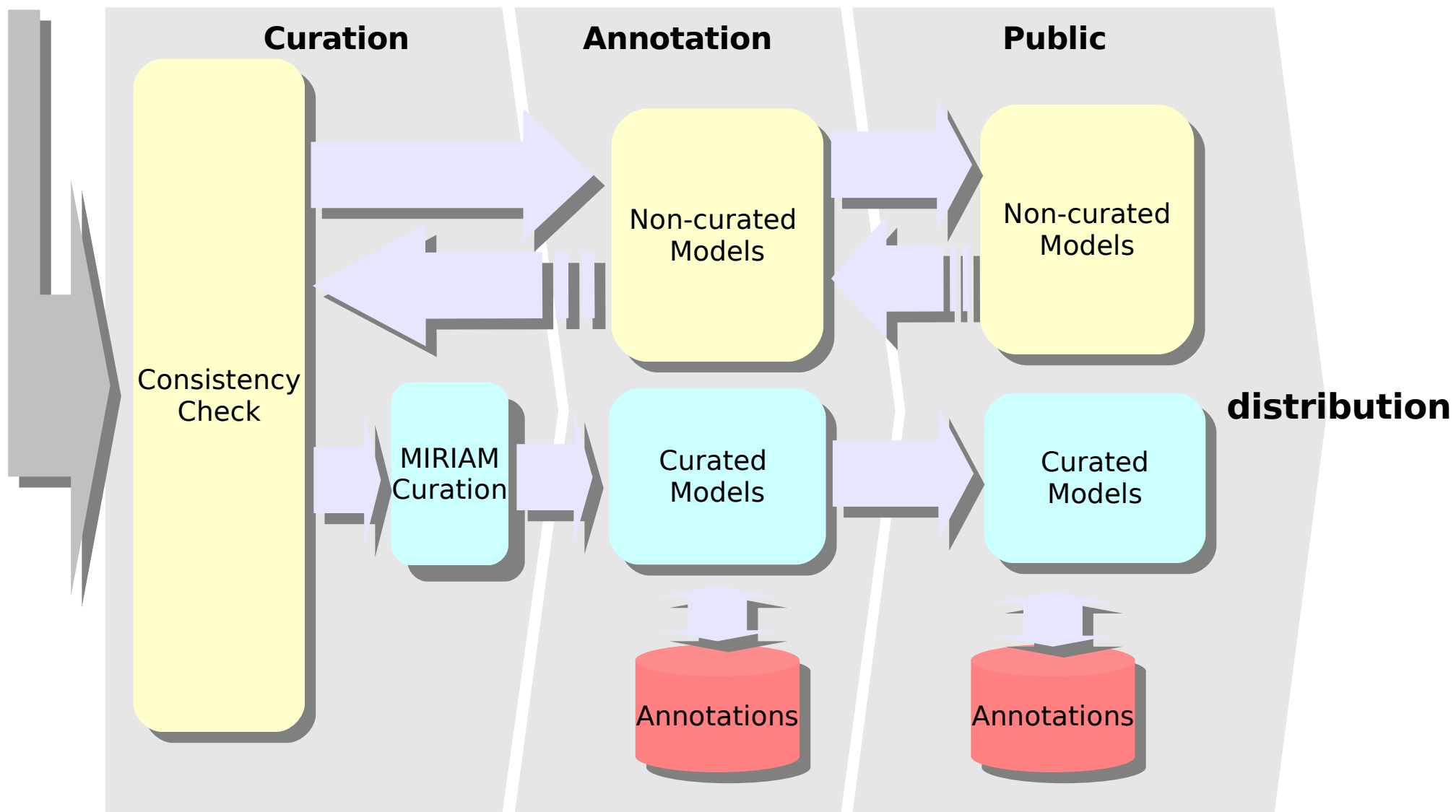
<http://www.ebi.ac.uk/biomodels/>



- Store and serve quantitative models of biomedical interest
- Only models described in the peer-reviewed scientific literature.
- Models are curated: computer software check the syntax, while human curators check the semantics.
- Models are simulated to check the reference correspondence
- Model components are annotated, to improve identification and retrieval.
- Models are accepted in several formats, and served in several others.
- Aims to be the “UniProt” of quantitative modelling.



Submission





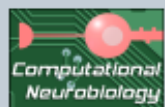
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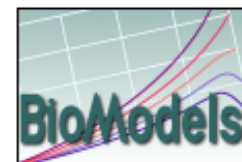
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BioModels Database

A Database of Annotated Published Models

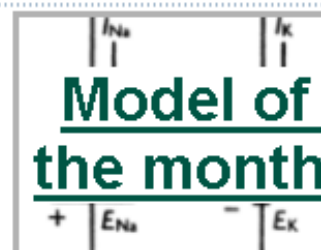
BioModels Database is a data resource that allows biologists to store, search and retrieve published mathematical models of biological interests. Models present in BioModels Database are annotated and linked to relevant data resources, such as publications, databases of compounds and pathways, controlled vocabularies, etc.


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[\[Browse non-curated models \]](#)
[\[Search \]](#)

3rd October 2006 - Sixth Release! [\[More\]](#) [\[Download All Models Under SBML L2 V1 Format\]](#)

July 2006 - PLoS Computational Biology supports BioModels Database [\[more\]](#)

06th January 2006 - publication of a paper describing BioModels Database [\[Nucleic Acids Res.\]](#)


[Acknowledgements](#)

BioModels Database is developed in collaboration by the teams of [Nicolas Le Novère](#) (EMBL-EBI, United-Kingdom), [Michael Hucka](#) ([SBML Team](#), Caltech, USA), [Herbert Sauro](#) (Keck Graduate Institute, USA), [Hiroaki Kitano](#) (Systems Biology Institute, Japan), [Hans Westerhoff](#) and [Jacky Snoep](#) ([JWS Online](#), Stellenbosch (ZA) and Manchester (UK) Universities and ZA), as part of the [BioModels.net](#) initiative. BioModels Database development has benefitted from funds of the [European Molecular Biology Laboratory](#) (Le Novère team) and the [National Institute of General Medical Sciences](#) (SBML team).

Developers: Mélanie Courtot, Arnaud Henry, Camille Laibe, Chen Li (main developer), Lu Li, Nicolas Rodriguez (Alumni: Marco Donizelli)

Model curators and annotators: Harish Dharuri, Henuo He, Nicolas Le Novère, Lu Li, Rainer Machne, Bruce Shapiro.

Summer Internships

We are looking for intern students to work on the curation of our BioModels Database. These internships are not part of a university training. Nevertheless, this is an opportunity for the postholders to gain experience in an international environment. A limited funding is provided to cover for living expenses.

Successful candidates have experience in working with GNU/Linux operating system, and have a good knowledge of the main data resources used in biology. Curation of BioModel Database requires solid bases of mathematics and a good knowledge of

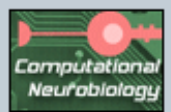
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- **BioModels ID** → Search BioModels Database for exact BioModels identifiers (for example *BIOMD0000000007* or *BIOMD0000000022*).
- **Person** → Search BioModels Database for model submitter and/or creator(s) names, or model reference publication author(s) names (for example *Nicolas Le Novère*, *Nicolas*, *Bruce Shapiro* or *Shapiro*, *Edelstein* or *Novak*).
- **SBML Elements** → Search BioModels Database for SBML elements by either name or *notes* content (for example *Edelstein* or *nicotinic*).
- **Resource** → Search BioModels Database for related information found in the models reference publication or third-party resources, by either publication/resource identifier or text (for example *9256450* or *cyclin* for publication, *GO:0007049* or *cell cycle* for Gene Ontology, *P04551* or *cell division* for UniProt).
- **Resource ID** → Search BioModels Database for annotations, by third-party resource identifiers (for example *IPR002394* for InterPro, *hsa04080* for KEGG Pathway, *68910* for Reactome).

A part from the *BioModels ID*-based search, for every other criteria the search operates on a *contains the entered string basis*, case-insensitive. That is, searching *Person* for *Shapi* or *shapi* will return the same results as searching for *Shapiro* or *shapiro*. In addition, since search strings are treated as words, do not enter regular expressions.

Multiple criteria can be combined with either *and* or *or*. If *and* is selected, only those models satisfying all the criteria will be returned. If instead *or* is selected, all the models satisfying at least one of the criteria will be returned.

BioModels ID:

Person:

SBML Elements:

Resource: Gene Ontology

Resource: Publication

Resource: ChEBI

Resource: Gene Ontology

Resource: Taxonomy

Resource ID: UniProt

Resource ID: BIND

Resource ID: BIND

Compose by: ☒ and ☐ or

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Last modification: Fri May 28 02:36:06 BST 2006

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Search Models

The search totally returned **13** models.

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Show 10 Only

13 Curated Models returned.

BioModels ID ▼	Name	Publication ID	Last Modified
BIOMD0000000009	Huang1996_MAPK_ultrasens	8816754	2006-09-30T23:18:39
BIOMD0000000010	Kholodenko2000_MAPK_feedback	10712587	2006-09-30T23:27:53
BIOMD0000000011	Levchenko2000_MAPK_noScaffold	10823939	2006-09-15T23:41:42
BIOMD0000000014	Levchenko2000_MAPK_Scaffold	10823939	2006-09-18T00:04:02
BIOMD0000000026	Markevich2004_MAPK_orderedElementary	14744999	2006-04-02T18:50:28
BIOMD0000000027	Markevich2004_MAPK_orderedMM	14744999	2006-08-14T13:52:32
BIOMD0000000028	Markevich2004_MAPK_phosphoRandomElementary	14744999	2006-04-02T18:53:13
BIOMD0000000029	Markevich2004_MAPK_phosphoRandomMM	14744999	2006-08-14T13:53:16
BIOMD0000000030	Markevich2005_MAPK_AllRandomElementary	14744999	2006-04-02T18:57:56
BIOMD0000000031	Markevich2004_MAPK_orderedMM2kinases	14744999	2006-04-02T18:58:15
BIOMD0000000032	Kofahl2004_pheromone	15300679	2006-08-20T01:25:41
BIOMD0000000033	Brown2004_NGF_EGF_signaling	14525003	2006-08-14T13:59:12
BIOMD0000000049	Sasagawa2005_MAPK	15793571	2006-08-24T23:29:11

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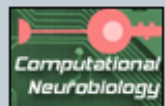
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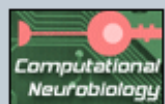
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Reference Publication

Publication ID: [10712587](#)

Eur J Biochem 2000 Mar;267(6):1583-8.
Negative feedback and ultrasensitivity can bring about oscillations in the mitogen-activated protein kinase cascades.
Kholodenko BN.
Department of Pathology, Anatomy and Cell Biology, Thomas Jefferson University, Philadelphia, PA 19107, USA. Boris.Kholodenko@mail.tju.edu [\[more\]](#)

Model

Original Model: *Unspecified*

bqbiol:isHomologTo set #1 **Reactome** [REACT_634](#)

Submitter: [Nicolas Le Novère](#)

bqbiol:is set #1 **Taxonomy** [Xenopus laevis](#)

Submission Date: 2005-09-13T13:39:02

bqbiol:isVersionOf set #1 **Gene Ontology** [MAPKKK cascade](#)

Last Modification Date: 2006-09-30T23:27:53

Creation Date: 2005-02-12T00:18:12

Creators: [Herbert Sauro](#)



Compartments (1)

Species (8)

Rules (0)

Reactions (10)

Events (0)



BIOMD0000000010 Kholodenko2000_MAPK_feedback

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- Non-curated Models
- Search

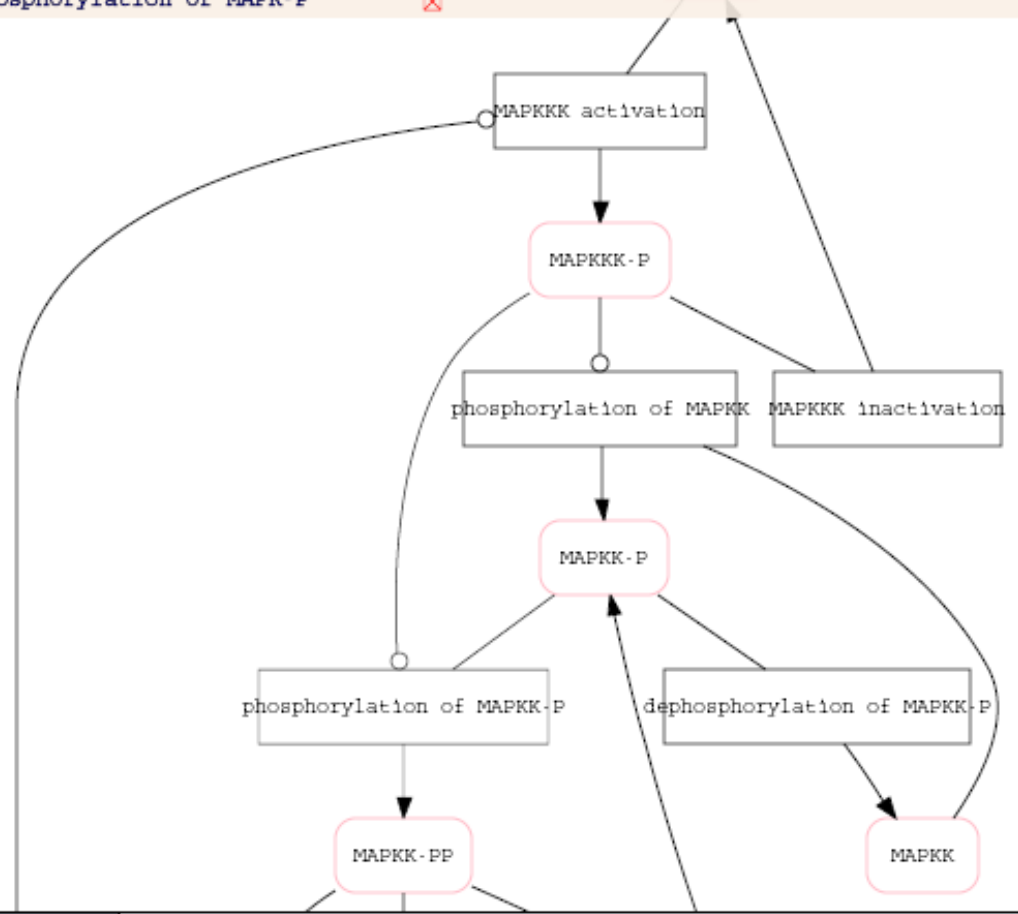
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http://www.ebi.ac.uk - SVG - Mozilla

Search For Species
Search For Reaction

MAPKKK activation	MAPKKK inactivation	phosphorylation of MAPKK
phosphorylation of MAPKK-P	dephosphorylation of MAPKK-PP	dephosphorylation of MAPKK-P
phosphorylation of MAPK	phosphorylation of MAPK-P	dephosphorylation of MAPK-PP
dephosphorylation of MAPK-P	⊗	



bout oscillations in the

ogy, Thomas Jefferson University,
@mail.tju.edu [\[more\]](#)

634

laevis

PKKK cascade

European Bioinformatics Institut...BioModels Database

Reactions (10)

MAPKKK activation

Reactants: MAPKKK

Products: MAPKKK-P

Modifiers: MAPK-PP

Referred to as: J0

MAPKKK inactivation

Reactants: MAPKKK-P

Products: MAPKKK

Modifiers:

Referred to as: J1

phosphorylation of MAPKK

Reactants: MAPKK

Products: MAPKK-P

Modifiers: MAPKKK-P

Referred to as: J2

phosphorylation of MAPKK-P

Reactants: MAPKK-P

Products: MAPKK-PP

Modifiers: MAPKKK-P

Referred to as: J3

dephosphorylation of MAPKK-PP

Reactants: MAPKK-PP

Products: MAPKK-P

Modifiers:

Referred to as: J4

dephosphorylation of MAPKK-P

Reactants: MAPKK-P

Products: MAPKK

Modifiers:

Referred to as: J5

phosphorylation of MAPK

Reactants: MAPK

Products: MAPK-P

Modifiers: MAPKK-PP

Referred to as: J6

bqbiol:is set #1

Gene Ontology activation of MAPKKK activity

Gene Ontology MAP kinase kinase kinase kinase activity

bqbiol:isVersionOf set #1

EC code 3.1.3

Gene Ontology

bqbiol:is set #1

Gene Ontology

bqbiol:isVersionOf set #1

EC code 2.7.1

Gene Ontology

bqbiol:is set #1

Gene Ontology

bqbiol:isVersionOf set #1

EC code 2.7.1

Gene Ontology

bqbiol:isVersionOf set #1

EC code 3.1.3

Gene Ontology

bqbiol:isVersionOf set #1

EC code 3.1.3

Gene Ontology

bqbiol:isVersionOf set #1

EC code 2.7.1.37

Gene Ontology protein amino acid phosphorylation

bqbiol:is set #1

Gene Ontology MAP kinase kinase activity

Reaction:

MAPKKK activation

rate law:

$$uVol * V1 * MAPKKK / ((1 + pow(MAPK-PP / K1, n)) * (K1 + MAPKKK))$$

Compartments

Name	Size
uVol	1.0

Species

Name	Compartment	Initial Amount	Initial Concentration
MAPKKK	uVol		90.0
MAPK-PP	uVol		10.0

Parameters

Name	Value
V1	2.5
K1	9.0
n	1.0
K1	10.0

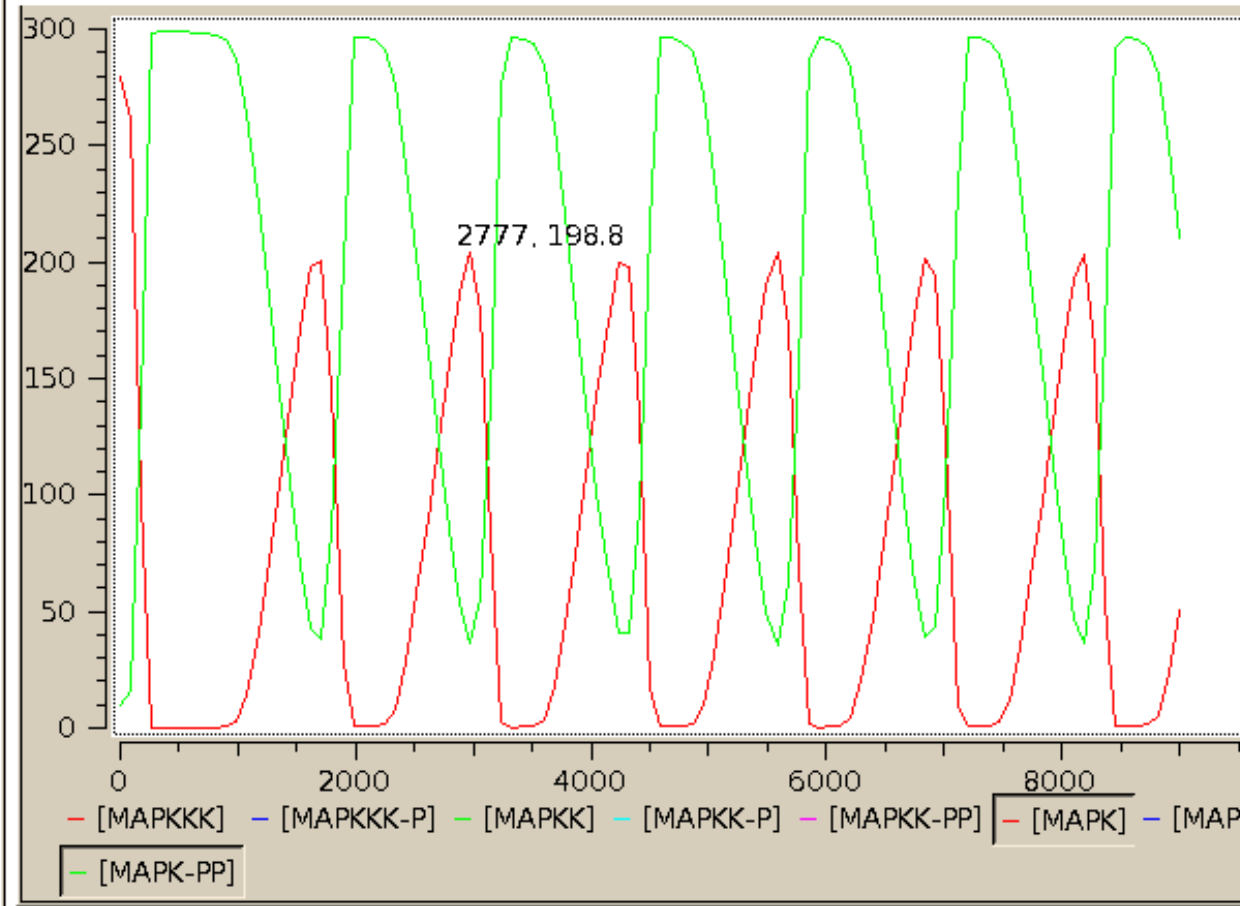
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Comment: Reproduction of figure 2a in COPASI 4.0 build 18

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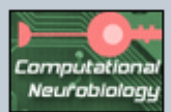
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gy, Thomas Jefferson University,
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B4

aevis

KKK cascade

000010')



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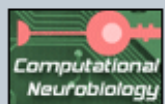
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Reference Publication

Publication ID: [10712587](#)

Eur J Biochem 2000 Mar;267(6):1583-8.
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Kholodenko BN.
Department of Pathology, Anatomy and Cell Biology, Thomas Jefferson University, Philadelphia, PA 19107, USA. Boris.Kholodenko@mail.tju.edu [\[more\]](#)

Model

Original Model: *Unspecified*

bqbiol:isHomologTo set #1 [Reactome REACT_634](#)

Submitter: [Nicolas Le Novère](#)

bqbiol:is set #1 [Taxonomy Xenopus laevis](#)

Submission Date: 2005-09-13T13:39:02

bqbiol:isVersionOf set #1 [Gene Ontology MAPKKK cascade](#)

Last Modification Date: 2006-09-30T23:27:53

Creation Date: 2005-02-12T00:18:12

Creators: [Herbert Sauro](#)



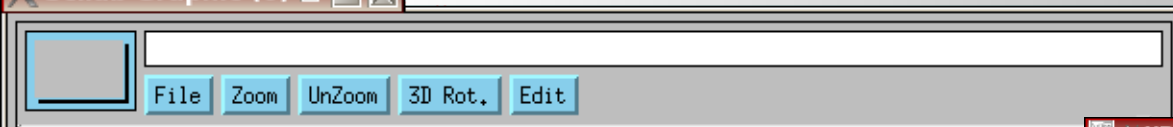
Compartments (1)

Species (8)

Rules (0)

Reactions (10)

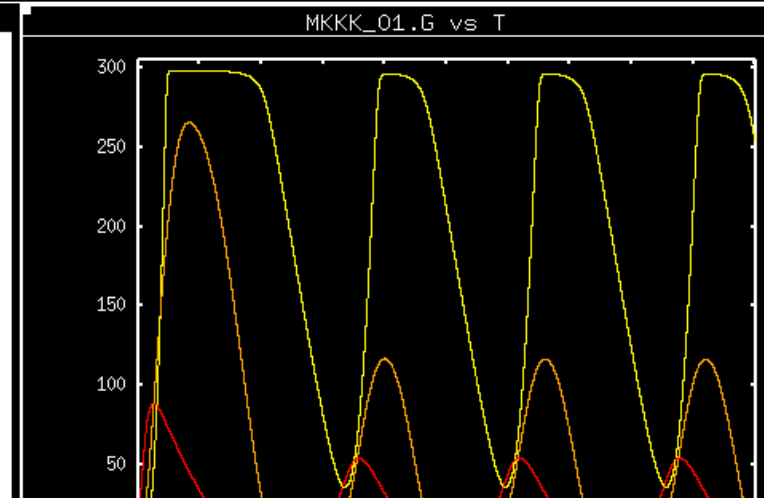
Events (0)



XPP Ver 5.85 >> BIOMD0000000010.xpp

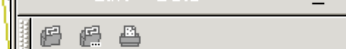
ICs BCs Delay Param Eqns Data

XPP
Initialconds
Continue
Nullcline
Dir.field/flow
Window/zoom
phAsespace
Kinescope
Graphic stuff
nUmeric
File
Parameters
Erase
Makewindow
Text,etc
Sing pts
Viewaxes
View



ControlPanel BIOMD0000000010.xml

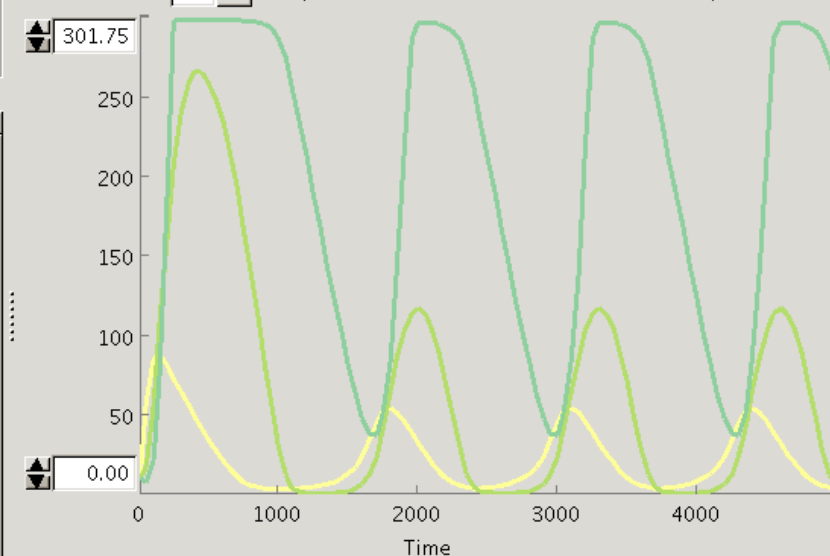
File Edit Data Simulation



Time span
End Tim 5,00
Num. of 100
Error tolerance
Exponent -6

Species Parameters Change

Id	Name	Compartment
MKKK	MAPKKK	uVol
MKKK_P	MAPKKK-P	uVol
MKK	MAPKK	uVol
MKK_P	MAPKK-P	uVol
MKK_PP	MAPKK-PP	uVol
MAPK	MAPK	uVol
MAPK_P	MAPK-P	uVol
MAPK_PP	MAPK-PP	uVol

Concentration raw ☒ Species ☐ Fluxes ☐ Parameters ☐ Compartments

Visib	Species	Co
☐	MAPKKK	
☒	MAPKKK	
☐	MAPKK	
☐	MAPKK-	
☒	MAPKK-	
☐	MAPK	
☐	MAPK-P	
☒	MAPK-P	

Select all

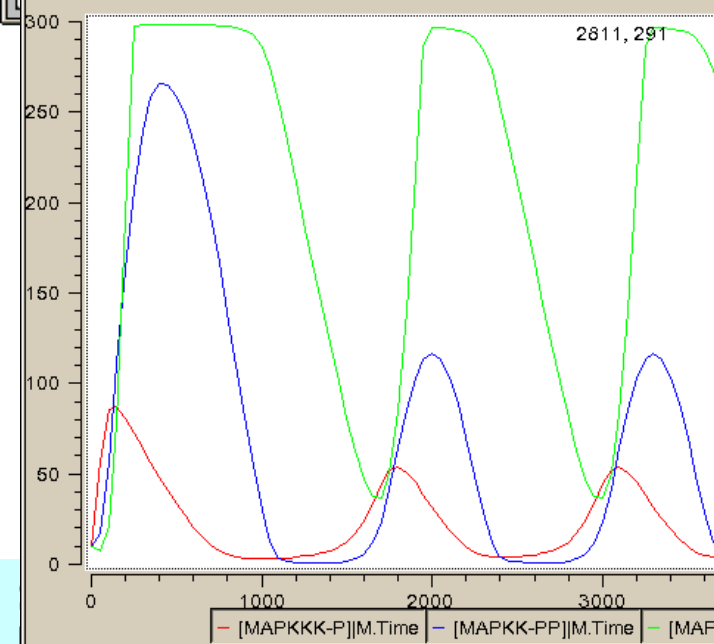
species search

search

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Search

Submit Your Model

Curation tips

Annotation tips

Sign-in

News

FAQ

Model of the month

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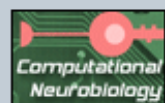
Related Software

Meetings

Contact

Quote

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MODEL8928994216	dAlesteros2002_SupersticDlasticity	12822459	2006-09-29T23:12:24

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Search

Submit Your Model

Curation tips

Annotation tips

Sign-in

News

FAQ

Model of the month

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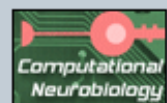
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Meetings

Contact

Quote

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News

FAQ

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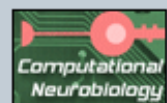
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Curation tips

Annotation tips

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News

FAQ

Model of the month

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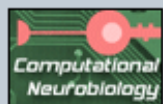
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MODEL8938994216	dAlesteros2002_Superelasticity	12822459	2006-09-29T23:12:24

I) Existing model repositories

- old SBML repository
- JWS Online
- Database Of Quantitative Cell Signalling
- CellML repository

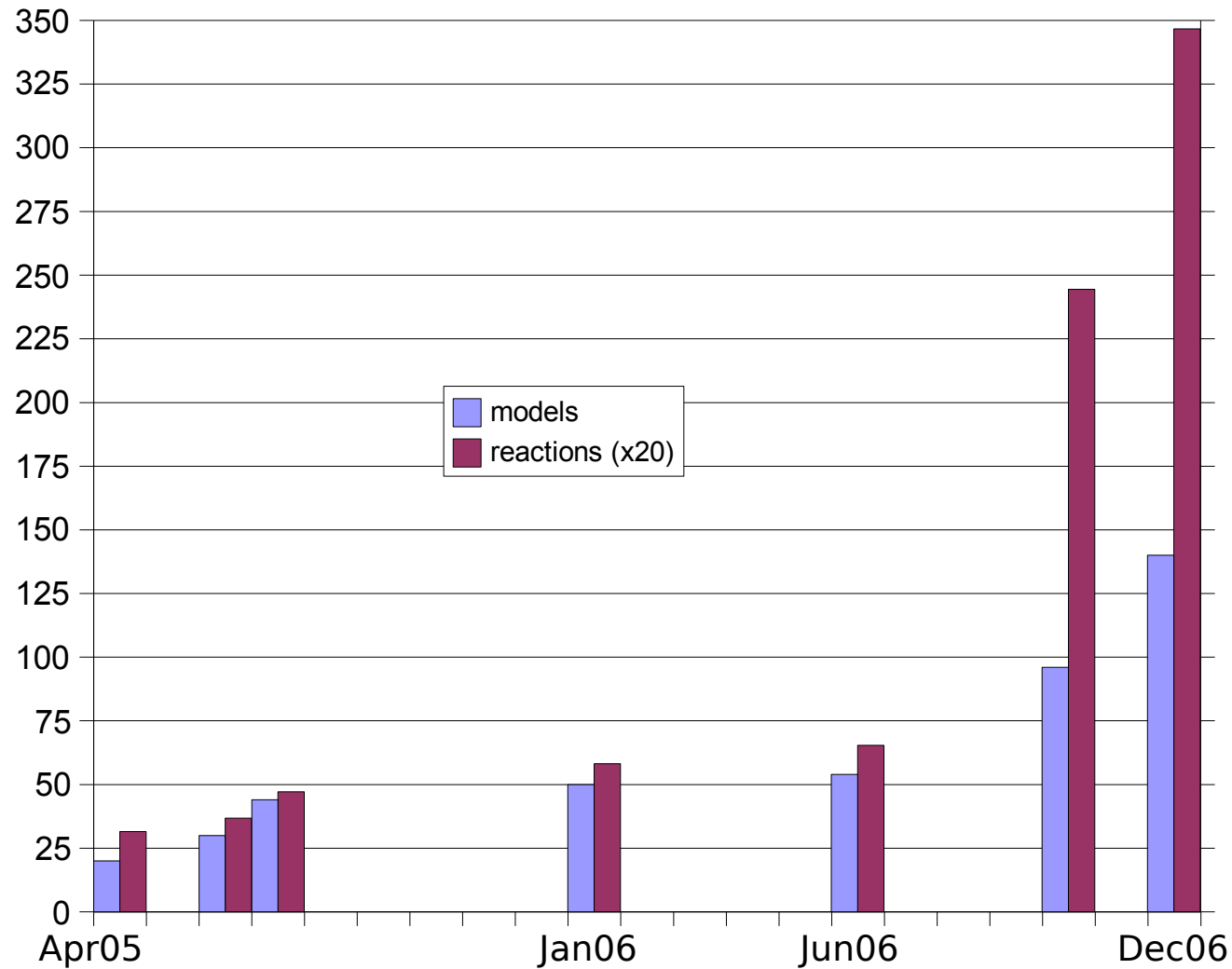
II) Individuals

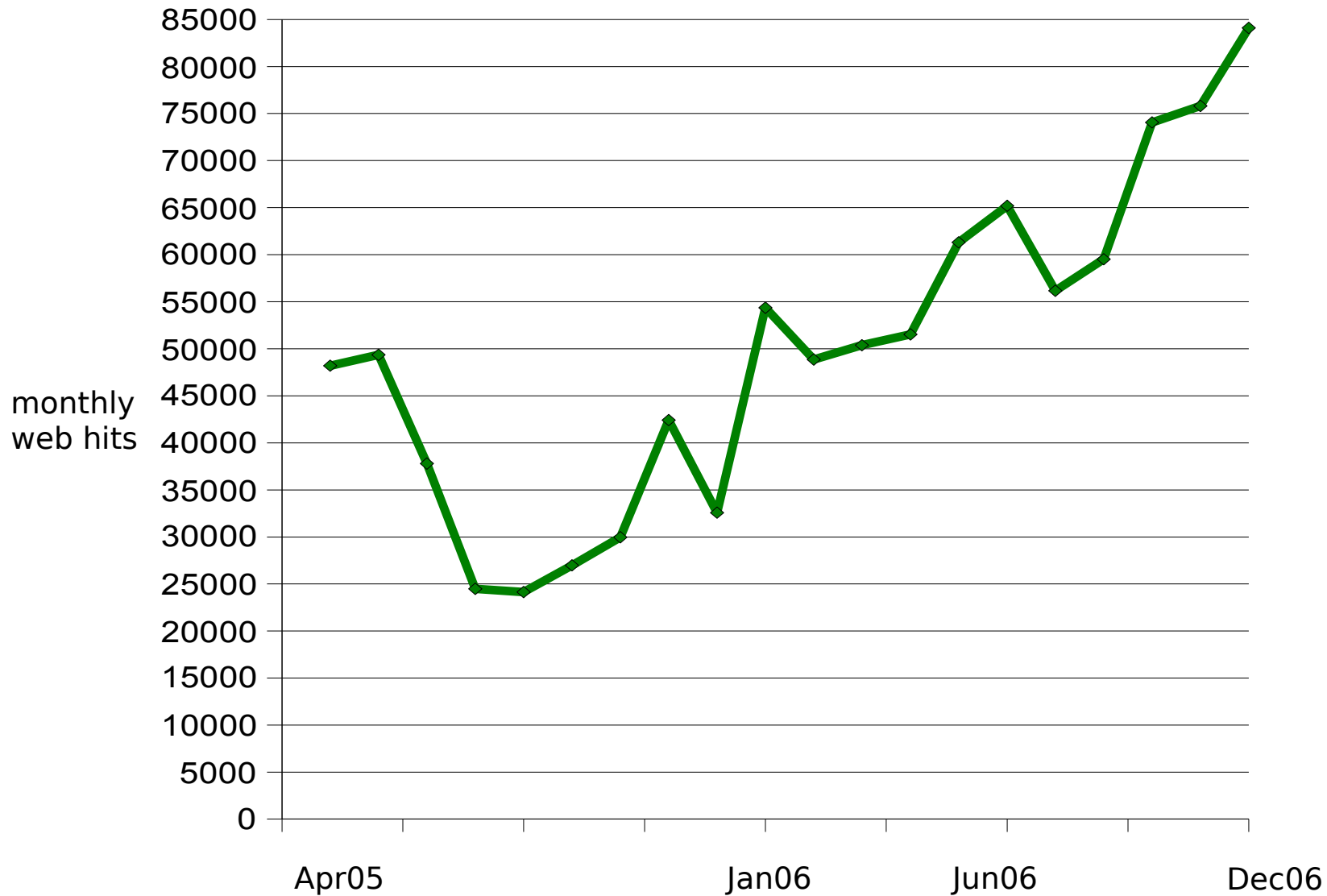
- Members of the SBML community (developers+modellers)
- Authors (prior to grant application, before publication etc.)

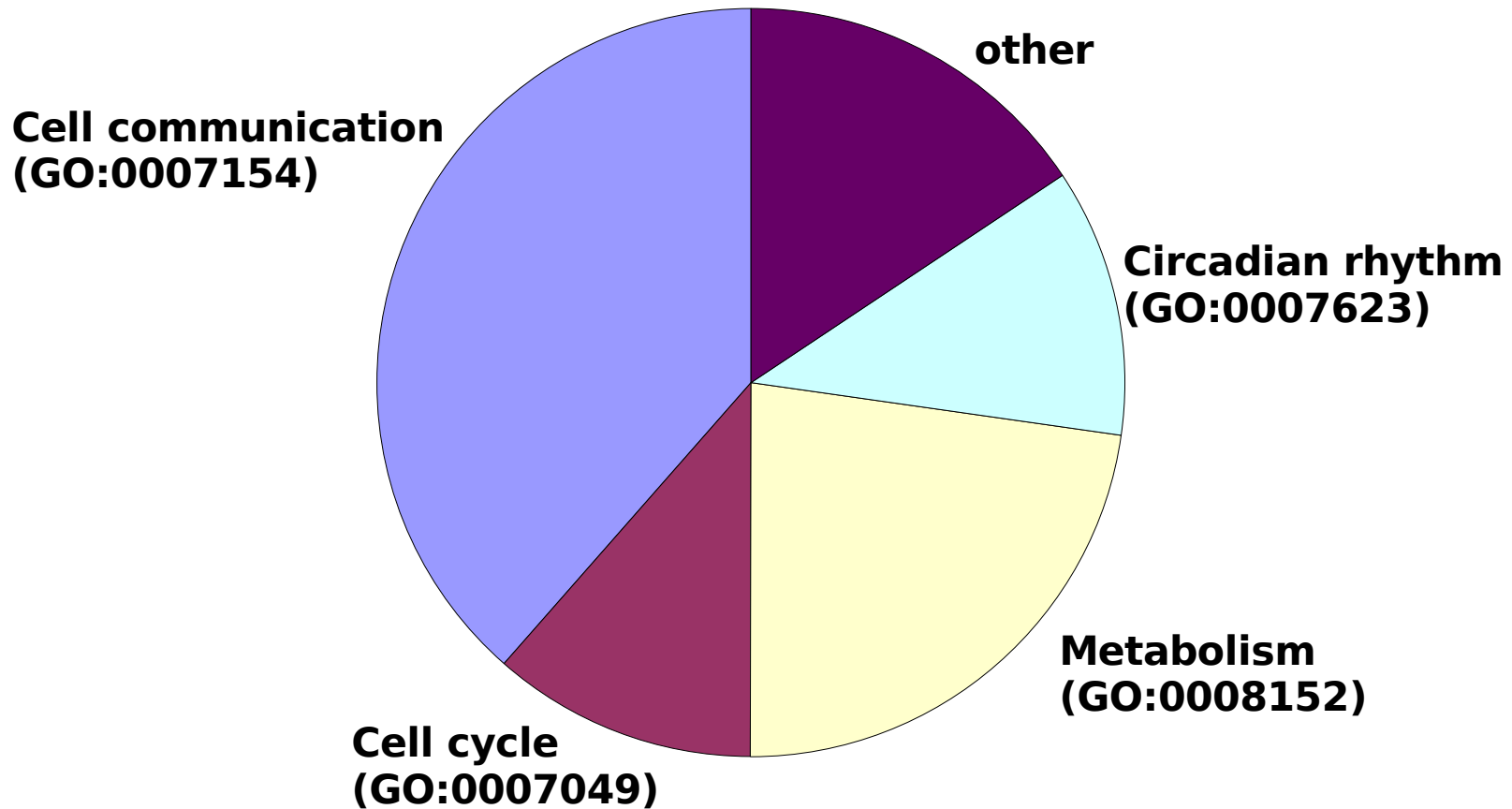
III) Journals (Molecular Systems Biology and PloS Computational Biology advise deposition)

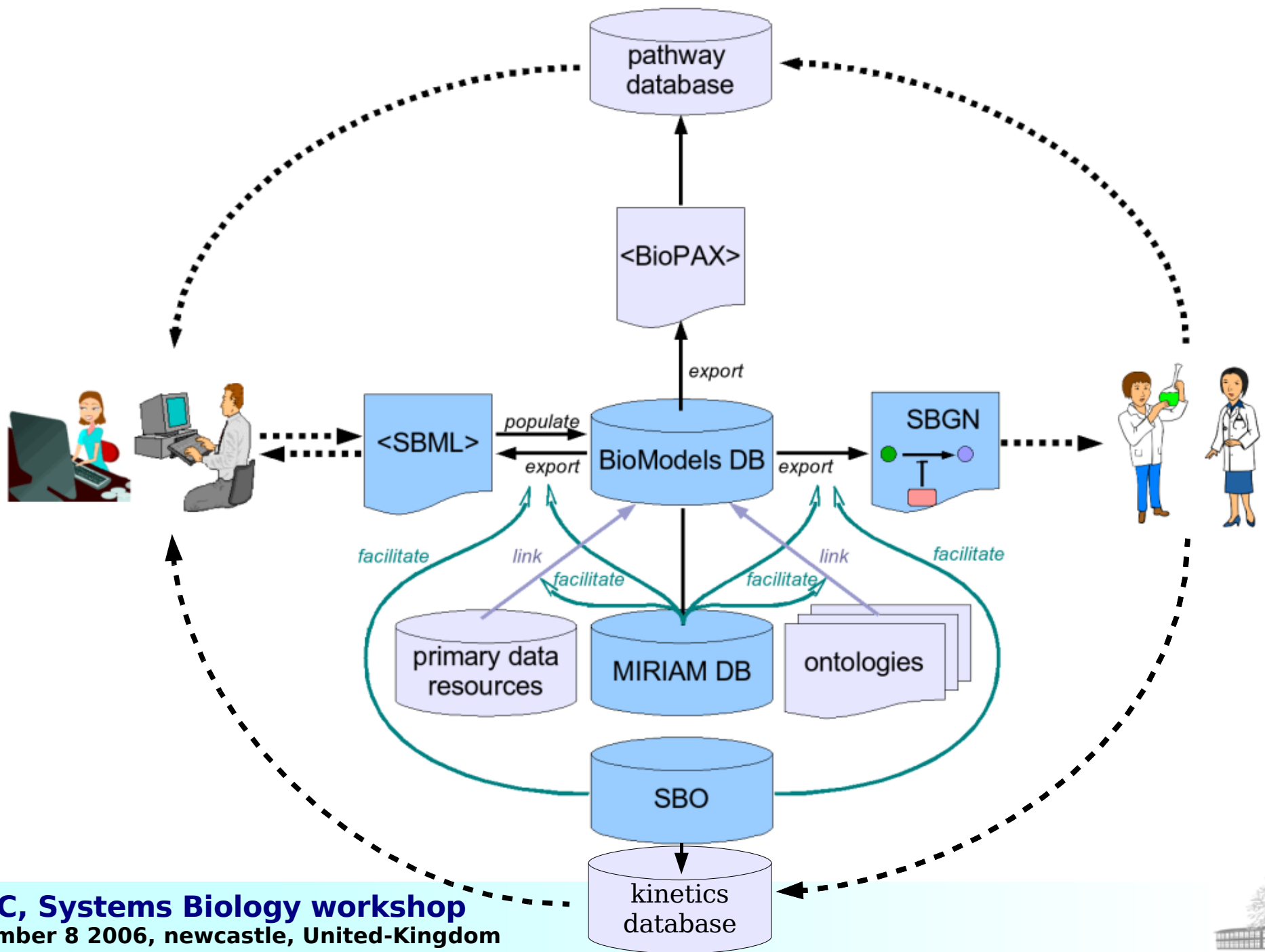
IV) BioModels DB curators encode new models from literature













Enuo He



Melanie Courtot



Nicolas
Le Novère



Lu Li



Chen Li



Harish
Dharuri



Camille Laibe

Marco Donizelli



Arnaud Henry



Michael
Hucka



EBI

- Nicolas Le Novère
- Marco Donizelli
- Chen Li
- Mélanie Courtot
- Lu Li
- Camille Laibe
- Arnaud Henry
- Enuo He
- Nicolas Rodriguez
- Alexander Broicher

SBML team

- Michael Hucka
- Andrew Finney
- Bruce Shapiro
- Benjamin Borstein
- Maria Schilstra
- Sarah Keating
- Harish Dharuri

NCBS

- Upinder Bhalla
- Harsha Rani

Keck Graduate Institute

- Herbert Sauro

Vienna TBI

- Rainer Machne

Systems Biology Institute

- Hiroaki Kitano
- Akira Funahashi

JWS Online

- Jacky Snoep
- Hans Westerhoff

Journals supporting BioModels Database

- Molecular Systems Biology
- PLoS Computational Biology

Programs used for curation

- CellDesigner/SBMLodeSolver
- COPASI
- Jarnac/JDesigner
- MathSBML
- SBMLeditor
- XPP-Aut

The community of Systems Biology for their contributions of models and comments.



British outstation of the European Molecular Biology Laboratory

- Databases

- Sequences, structures
- Transcriptomics, Proteomics pathways, models
- Controlled vocabularies and dictionaries



- Research groups

- Structural Genomics (Thornton)
- Molecular Evolution (Goldman)
- Text-Mining (Rebholz-Schumman)
- Computational Systems Biology (Le Novère)
- Statistical array analysis (Huber)
- Genomic analysis of regulatory systems (Luscombe)
- Systems Biology of ES cells (Bertone)

**Marie Curie Training site Fellowships: PhD 3-6 months. Fully funded.
Undergraduate trainees: 5-6 months.**