CSim & JSim

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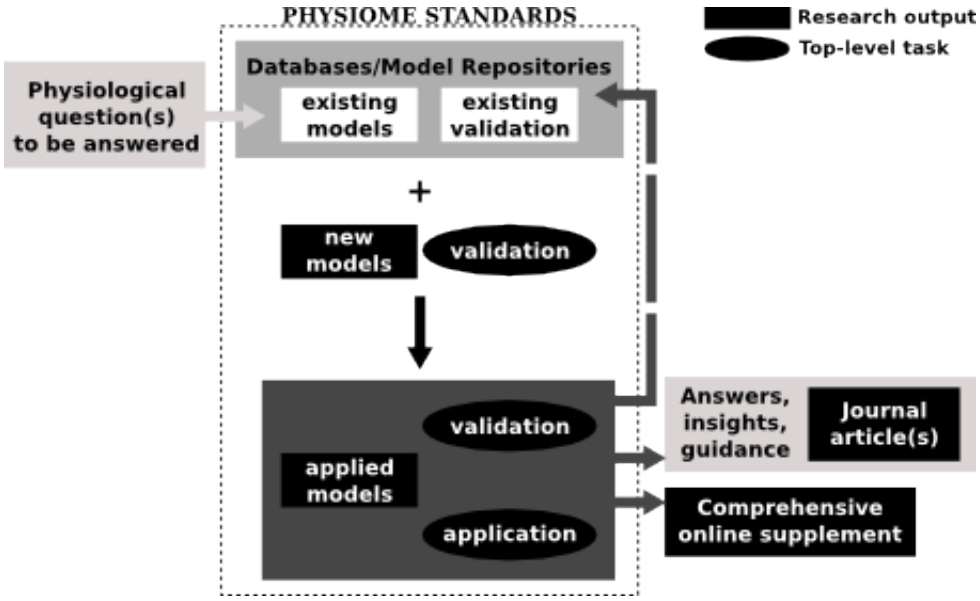
CellML Workshop 2012

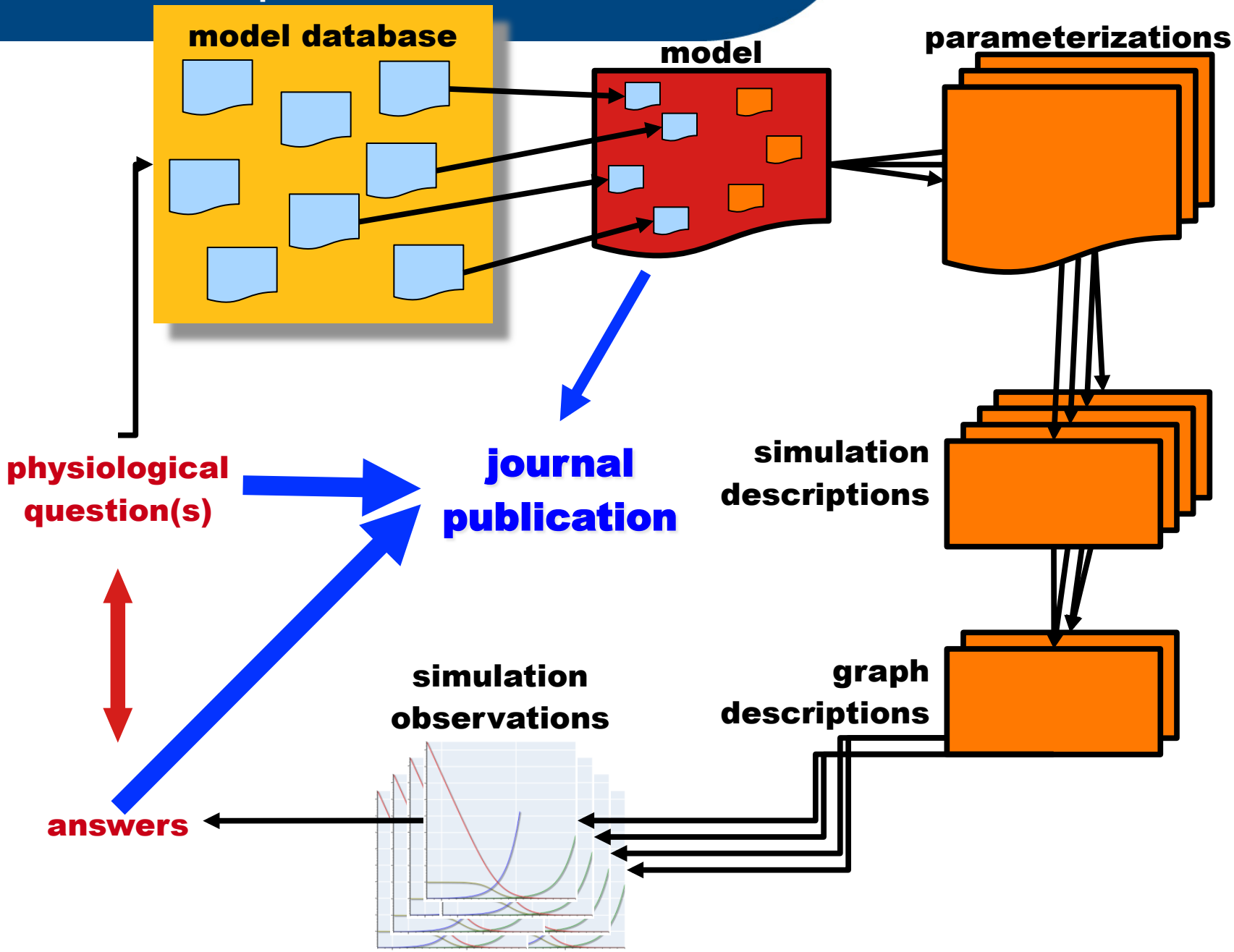
AUCKLAND
BIOENGINEERING INSTITUTE
THE UNIVERSITY OF AUCKLAND
NEW ZEALAND
Te Whare Wānanga o Tāmaki Makaurau

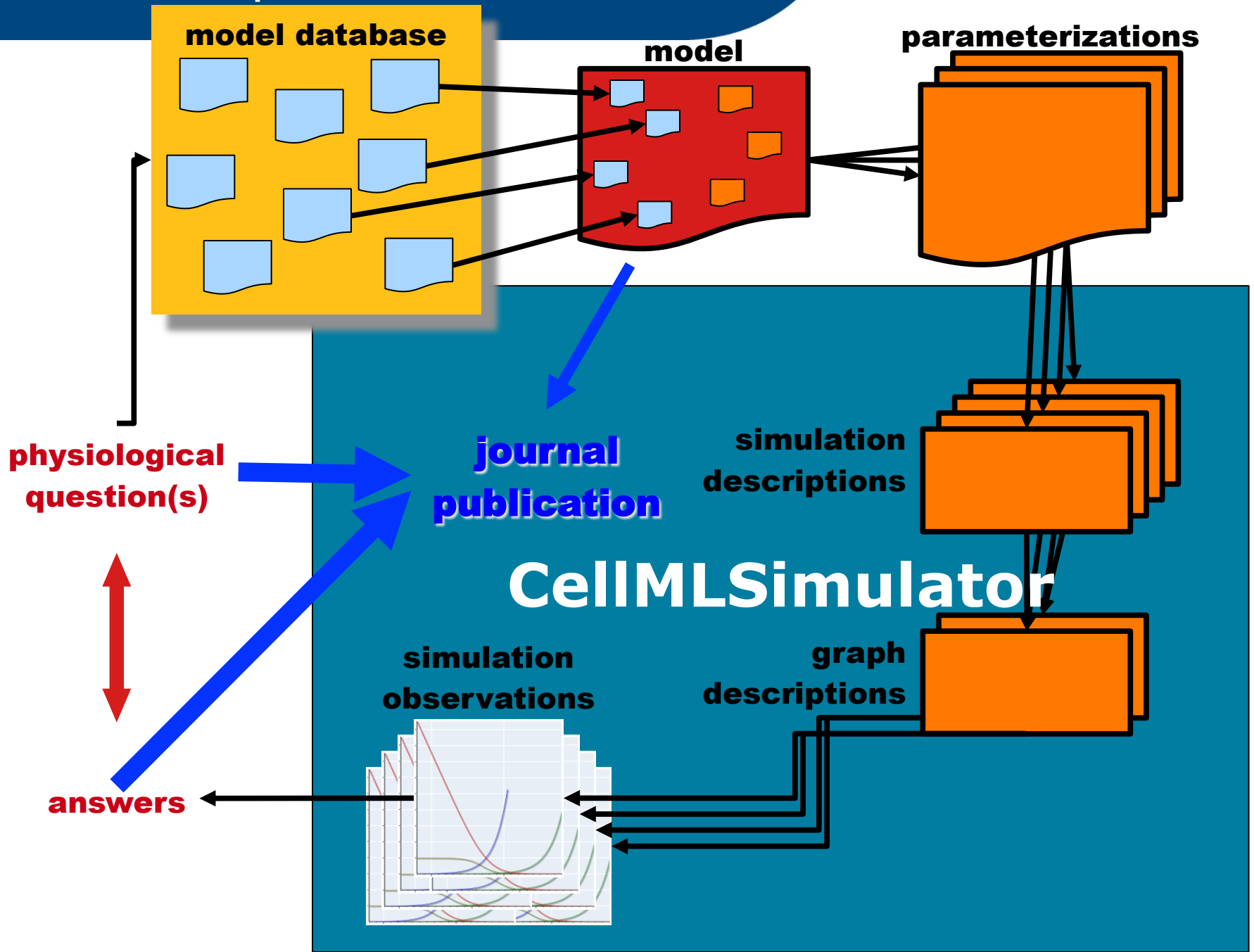
What is CSim?

- c-sim?
- Csim?
- cSim?

Paradigm summary




model database
model
parameterizations
physiological question(s)
journal publication
simulation descriptions
graph descriptions
simulation observations
answers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CellMLSimulator
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answers

Reference Description of a HH-based Modelling Study - Mozilla Firefox

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Reference Description of a HH-based Modelling Study

David Nickerson (2008-07-16)

Help

- Reference Description of a HH-based Modelling Study
  - Model Validation
    - Sodium Channel Kinetics Validation
      - INa Gating Rates
      - INa Steady State Gating Kinetics
    - Potassium Channel Kinetics Validation
      - IK Gating Rates
      - IK Steady State Gating Kinetics
    - Voltage Clamp Validation
    - Action Potential Validation
      - Action Potentials
      - Membrane Currents
      - Gating Variables
      - Action Potential
      - Membrane Currents
      - Gating Variables
  - The effect of membrane conductance
    - Sodium channel conductance
      - Action Potentials
      - Sodium current
    - Potassium channel conductance
      - Action Potentials
      - Potassium current
    - Leakage current conductance
      - Action Potentials
      - Leak current
    - Comparison of changes
      - Action Potentials - 50%
      - Action Potentials - 150%
      - Action Potentials - 200%
  - Varying ion concentrations
    - Changing Sodium
    - Changing Potassium
    - Changing Leakage

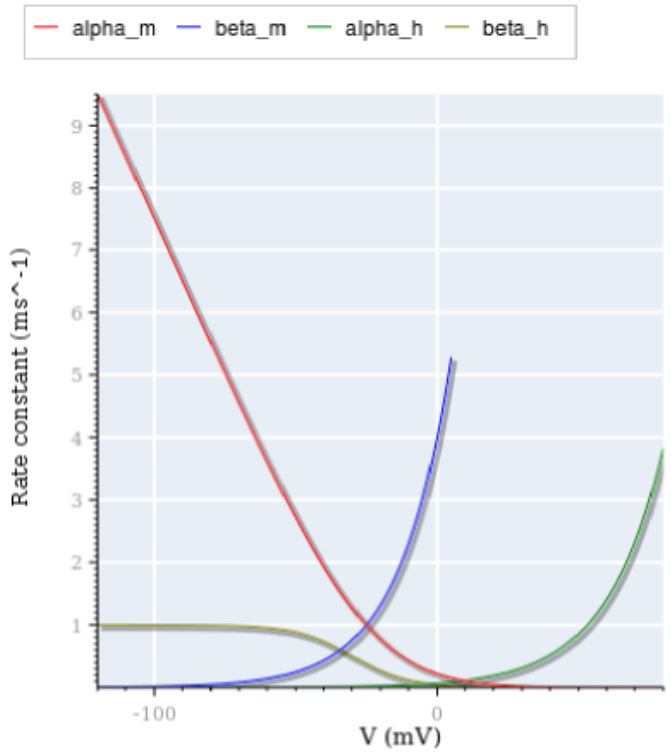
INa Gating Rates

+ A L HODGKIN & A F HUXLEY (1952)
+ Last modified: 2008-08-13, David Nickerson ()

Species: *loligo*

Biological Entity: giant nerve fibre

This graph matches Figures 7 and 9 of the Hodgkin & Huxley (1952) article.



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simulation
alpha

beta_h
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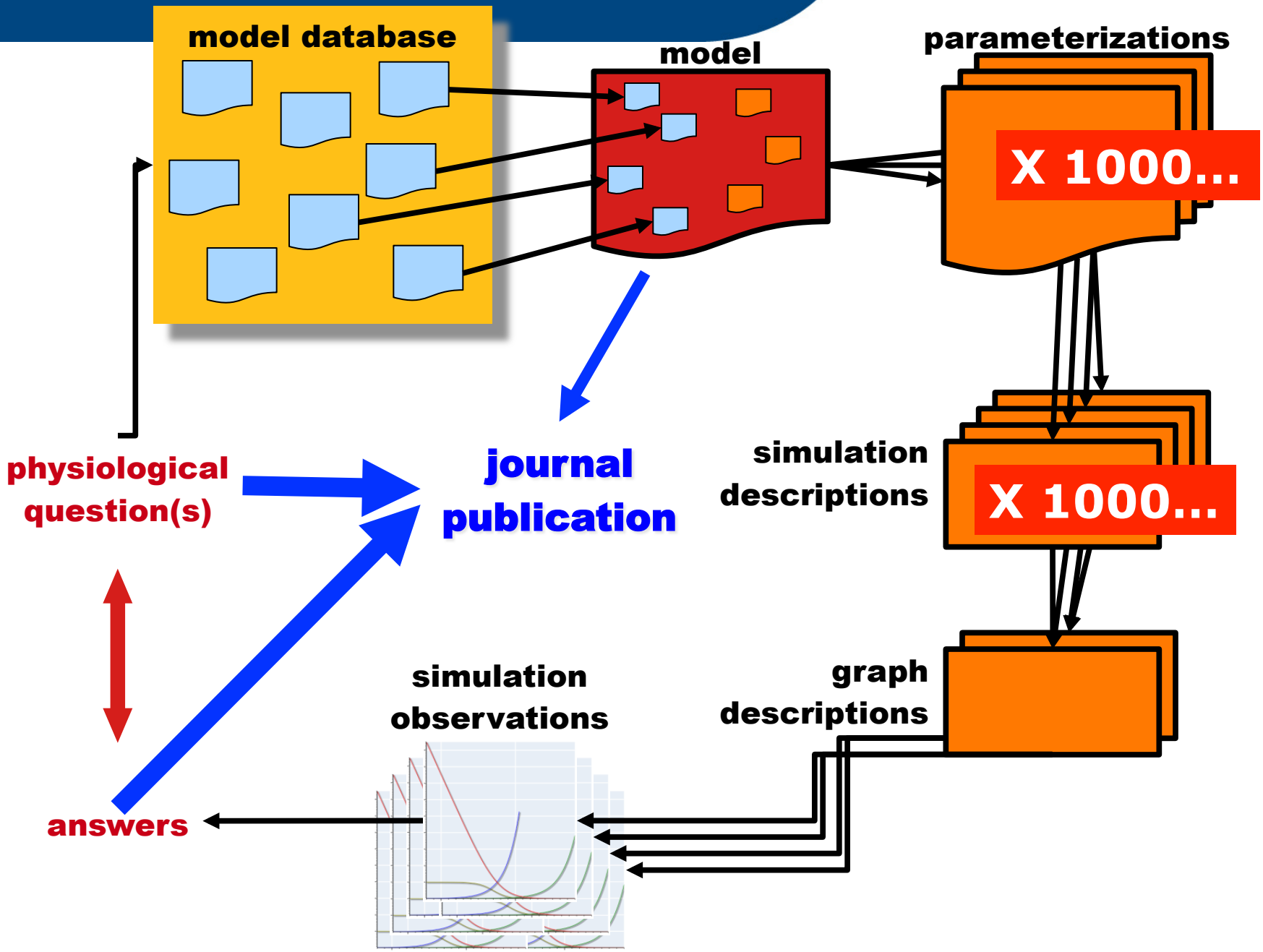
Generated by: CellMLSimulator (version: CellMLSimulator 0.3.0-devel-json - revision 132M - Thu Aug 14 18:14:54 SGT 2008) at Monday 01,September,2008 04:11:05 PM SGT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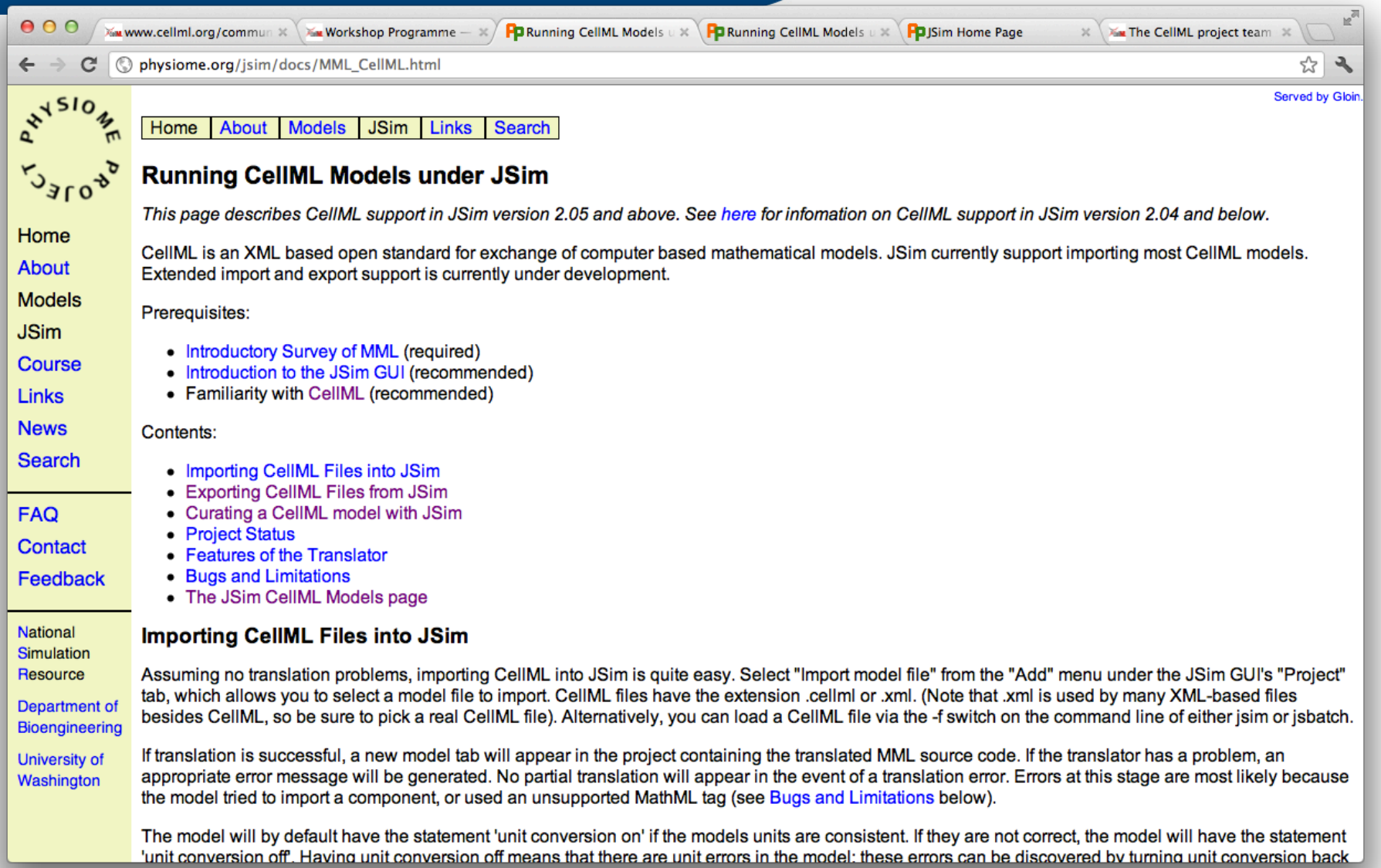
What is CSim?

- A simple command line application for running simulations based on CellML models – for this model integrate from X to Y outputting these variables every Z steps.
- Slots into existing SED-ML workflows as a CellML specific simulation tool – make use of generic SED-ML tools to perform model preprocessing and data analysis.
- Designed to be completely self-contained with no reliance on host system - just what is needed to easily ship simulations off to the cloud.

JSim

- No relation to CSim ☺
- Java-based simulation system for building quantitative numeric models and analyzing them with respect to experimental reference data.
- http://physiome.org/jsim/
- JSim's CellML importer has recently been substantially improved (thanks to Lucian Smith). JSim now runs 95% of the CellML 1.0 models in the CellML model repository out of box (no editing required).
- Good documentation on using JSim with CellML models: http://physiome.org/jsim/docs/MML_CellML.html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The CellML project team
physiome.org/jsim/docs/MML_CellML.html
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Running CellML Models under JSim
This page describes CellML support in JSim version 2.05 and above. See here for infomation on CellML support in JSim version 2.04 and below.
CellML is an XML based open standard for exchange of computer based mathematical models. JSim currently support importing most CellML models. Extended import and export support is currently under development.
Prerequisites:
Introductory Survey of MML (required)
Introduction to the JSim GUI (recommended)
Familiarity with CellML (recommended)
Contents:
Importing CellML Files into JSim
Exporting CellML Files from JSim
Curating a CellML model with JSim
Project Status
Features of the Translator
Bugs and Limitations
The JSim CellML Models page
Importing CellML Files into JSim
Assuming no translation problems, importing CellML into JSim is quite easy. Select "Import model file" from the "Add" menu under the JSim GUI's "Project" tab, which allows you to select a model file to import. CellML files have the extension .cellml or .xml. (Note that .xml is used by many XML-based files besides CellML, so be sure to pick a real CellML file). Alternatively, you can load a CellML file via the -f switch on the command line of either jsim or jsbatch.
If translation is successful, a new model tab will appear in the project containing the translated MML source code. If the translator has a problem, an appropriate error message will be generated. No partial translation will appear in the event of a translation error. Errors at this stage are most likely because the model tried to import a component, or used an unsupported MathML tag (see Bugs and Limitations below).
The model will by default have the statement 'unit conversion on' if the models units are consistent. If they are not correct, the model will have the statement 'unit conversion off'. Having unit conversion off means that there are unit errors in the model; these errors can be discovered by turning unit conversion back
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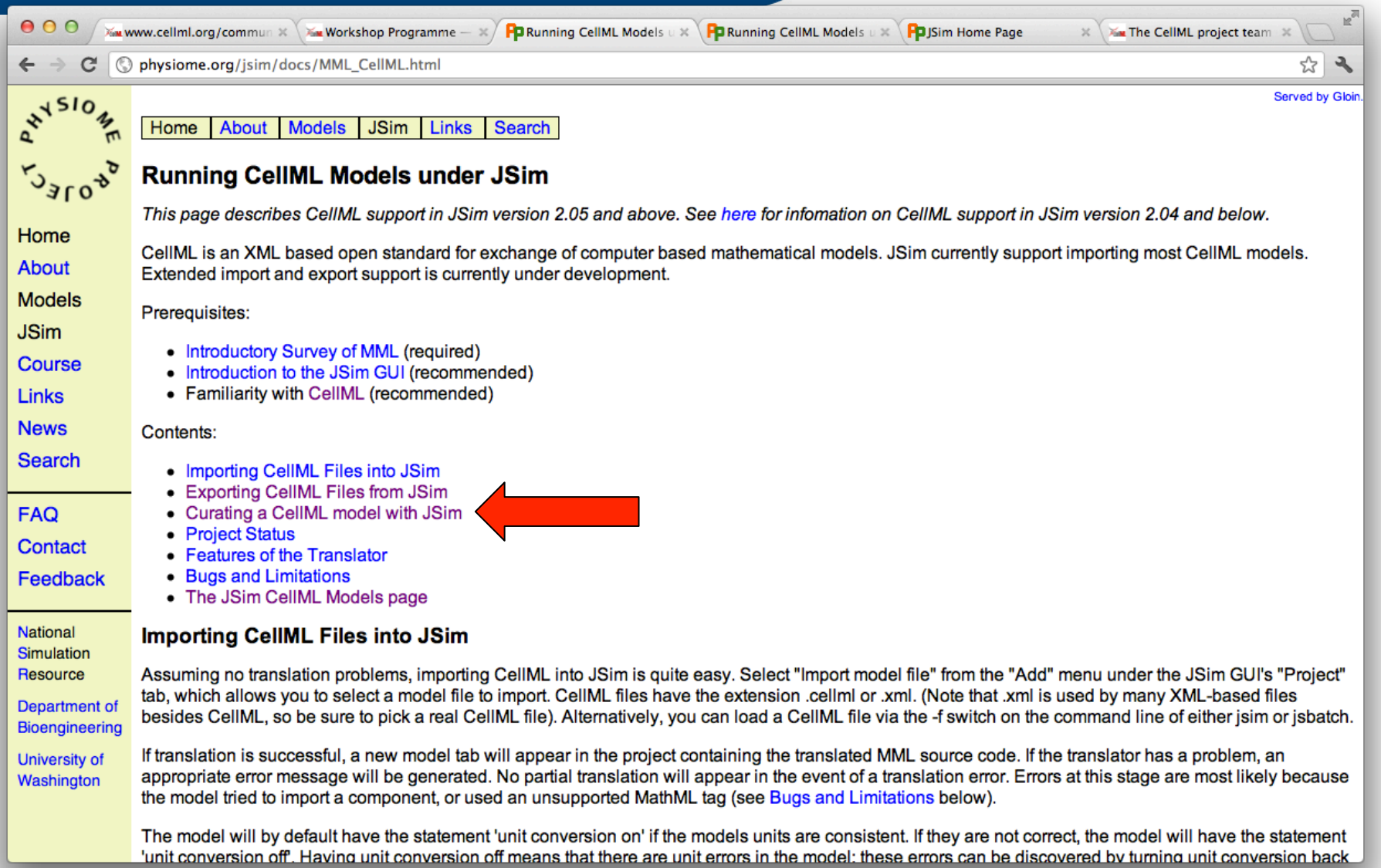
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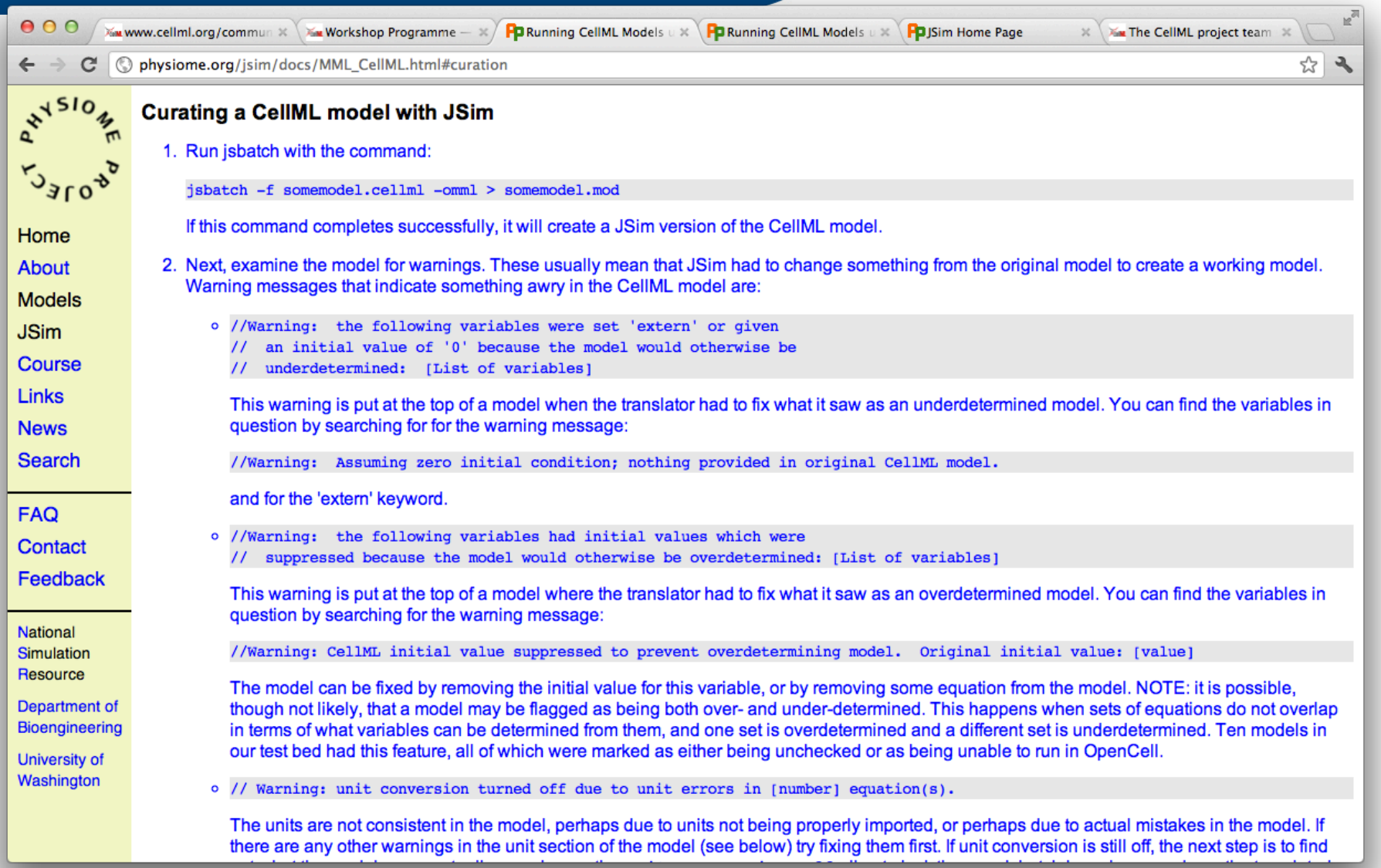
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Curating a CellML model with JSim
1. Run jsbatch with the command:
jsbatch -f somemodel.cellml -omml > somemodel.mod
If this command completes successfully, it will create a JSim version of the CellML model.
2. Next, examine the model for warnings. These usually mean that JSim had to change something from the original model to create a working model. Warning messages that indicate something awry in the CellML model are:
//Warning: the following variables were set 'extern' or given
// an initial value of '0' because the model would otherwise be
// underdetermined: [List of variables]
This warning is put at the top of a model when the translator had to fix what it saw as an underdetermined model. You can find the variables in question by searching for for the warning message:
//Warning: Assuming zero initial condition; nothing provided in original CellML model.
and for the 'extern' keyword.
//Warning: the following variables had initial values which were
// suppressed because the model would otherwise be overdetermined: [List of variables]
This warning is put at the top of a model where the translator had to fix what it saw as an overdetermined model. You can find the variables in question by searching for the warning message:
//Warning: CellML initial value suppressed to prevent overdetermining model. Original initial value: [value]
The model can be fixed by removing the initial value for this variable, or by removing some equation from the model. NOTE: it is possible, though not likely, that a model may be flagged as being both over- and under-determined. This happens when sets of equations do not overlap in terms of what variables can be determined from them, and one set is overdetermined and a different set is underdetermined. Ten models in our test bed had this feature, all of which were marked as either being unchecked or as being unable to run in OpenCell.
// Warning: unit conversion turned off due to unit errors in [number] equation(s).
The units are not consistent in the model, perhaps due to units not being properly imported, or perhaps due to actual mistakes in the model. If there are any other warnings in the unit section of the model (see below) try fixing them first. If unit conversion is still off, the next step is to find