Describing Mathematical Models of Cellular Physiology

David Nickerson & Martin Buist

NUS National University of Singapore

The Problem

- Mathematical models used in biology are getting more realistic.
- Traditional peer-reviewed articles rarely contain enough information to accurately reproduce or validate future model implementations.
- Required information often buried in complex computational code.
- Quantitative validation is generally impossible without full cooperation of original authors.

The Answer

- Encode mathematical models in standard formats.
- Unambiguously annotate the encoded model with as much information as possible, preferably using community defined standard annotations.
- Develop tools capable of rendering the annotated models into a human readable format.
- Integrate such annotated models into the model development and publication workflows.

Our solution

- **Encode models in CellML.**
- Use standard CellML Metadata for base annotation with the goal being MIRIAM compliance at the minimum.
- CellML Simulation metadata to annotate specific "*experiments*" with numerical methods data.
- CellML Graphing metadata to collate and extract specific numerical data from multiple "*experiments*", as well as provide the connection to experimental data.

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CellML Metadata

- **Combination of existing standards plus CellML specific data to fill in the gaps**
  - RDF from the W3C Semantic Web;
  - Dublin Core Metadata Initiative;
  - vCard to describe people;
  - Bibliographic Query Service.
- **CellML Metadata adds biology-related attributes and various missing properties.**

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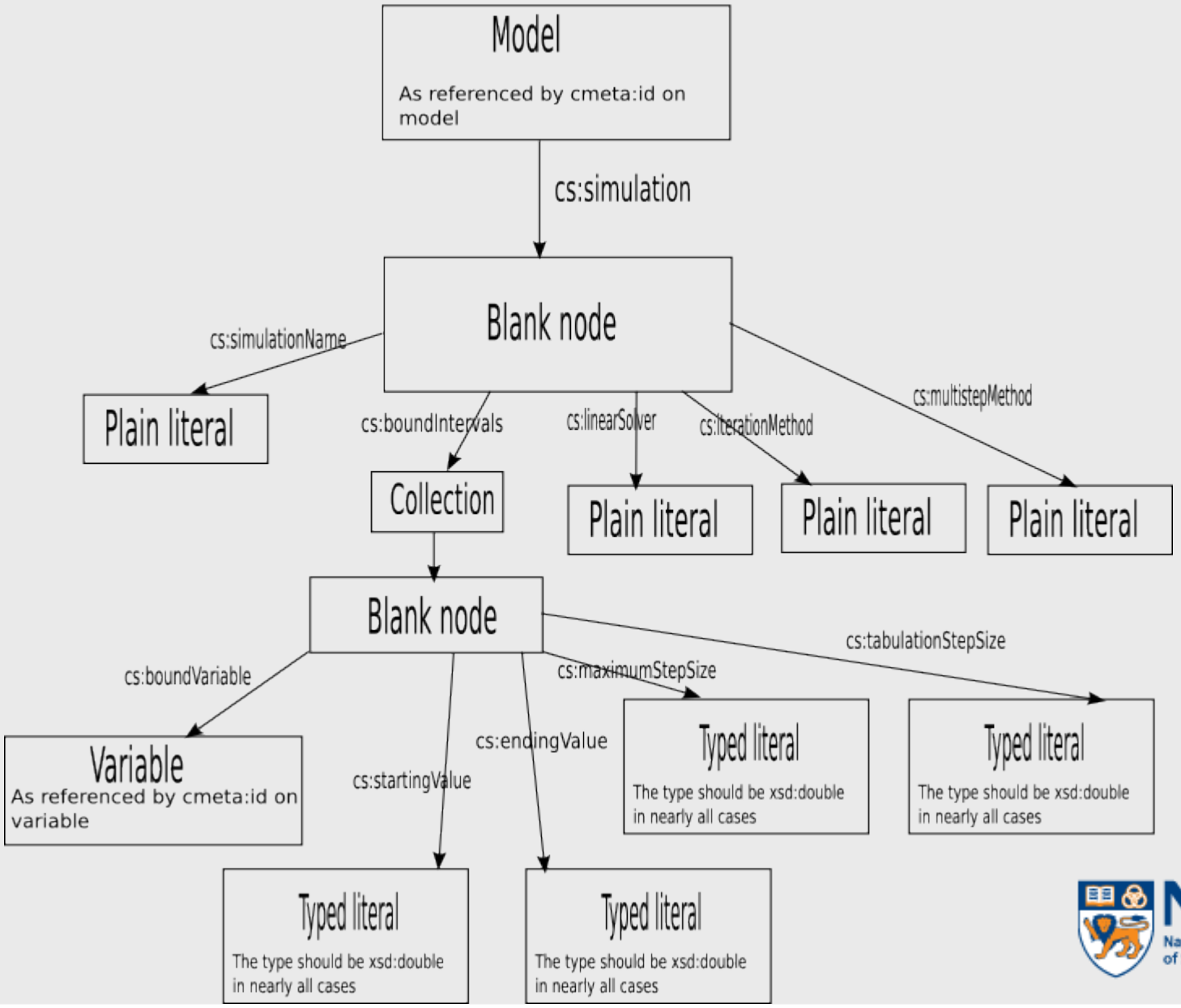
Note: Prefix cs: refers to http://www.cellml.org/metadata/simulation/1.0#
Prefix cmeta: refers to http://www.cellml.org/metadata/1.0#



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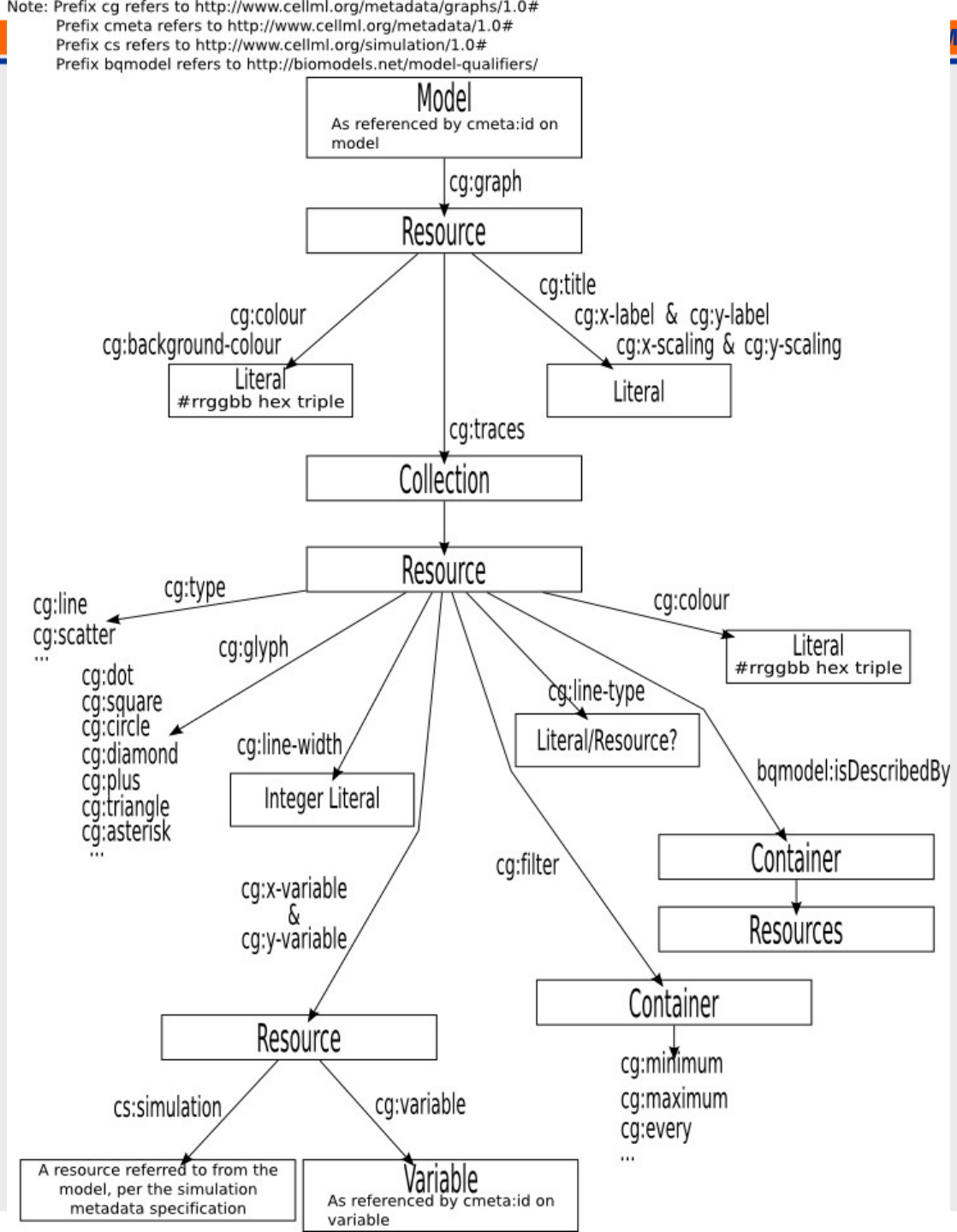
Note: Prefix cg refers to http://www.cellml.org/metadata/graphs/1.0#
Prefix cmeta refers to http://www.cellml.org/metadata/1.0#
Prefix cs refers to http://www.cellml.org/simulation/1.0#
Prefix bqmodel refers to http://biomodels.net/model-qualifiers/
Model
As referenced by cmeta:id on model
cg:graph
Resource
cg:colour
cg:background-colour
Literal
#rrggbb hex triple
cg:title
cg:x-label & cg:y-label
cg:x-scaling & cg:y-scaling
Literal
cg:traces
Collection
Resource
cg:type
cg:line
cg:scatter
...
cg:glyph
cg:dot
cg:square
cg:circle
cg:diamond
cg:plus
cg:triangle
cg:asterisk
...
cg:line-width
Integer Literal
cg:line-type
Literal/Resource?
cg:colour
Literal
#rrggbb hex triple
bqmodel:isDescribedBy
Container
Resources
cg:filter
cg:x-variable
&
cg:y-variable
Container
cg:minimum
cg:maximum
cg:every
...
Resource
cs:simulation
cg:variable
A resource referred to from the model, per the simulation metadata specification
Variable
As referenced by cmeta:id on variable

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- CellML Simulation metadata to annotate specific "*experiments*" with numerical methods data.
- CellML Graphing metadata to collate and extract specific numerical data from multiple "*experiments*", as well as provide the connection to experimental data.

Reference descriptions of cellular electrophysiology models
David P Nickerson, Alberto Corrias, & Martin L Buist
***Bioinformatics* 2008; doi: 10.1093/bioinformatics/btn080**

http://www.bioeng.nus.edu.sg/compbiolab/p2

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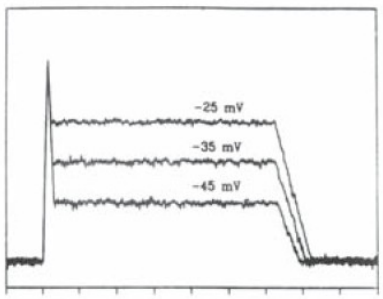
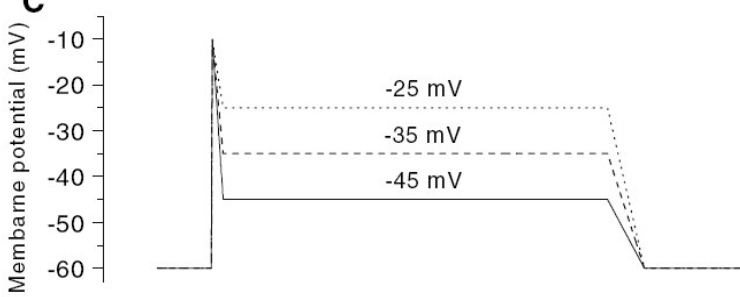
file:///home/...example-2.xml The Hodgkin & Huxley (195...





Applied Voltage Clamp Protocol

Creator: David Nickerson (david.nickerson@nus.edu.sg) Division of Bioengine

Created: 2007-09-11

Publisher: Division of Bioengineering, National University of Singapore

Pubmed reference: 17486452

Comment [created by David Nickerson (david.nickerson@nus.edu.sg) Division of Bioengineering, National University of Singapore]:

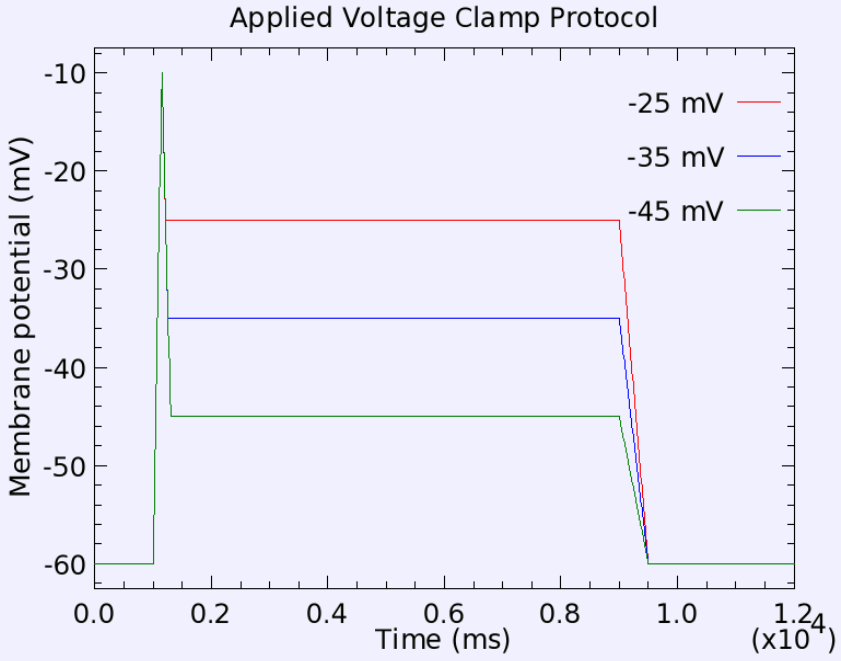
This graph partially provides a reproduction of Figure 2(C) from Corrias & Buist (2007).

Created: 2007-11-22

Modification [modified by David Nickerson (david.nickerson@nus.edu.sg) Division of Bioengineering, National University of Singapore]:

Adding standard CellML metadata annotations to the graph descriptions.

Modified: 2007-11-22



-25 mV

x-axis

Simulation: ...tage-clamp-25mV.xml#simulation

Variable: ...nts/ICa-voltage-clamp.xml#time

y-axis

Simulation: ...tage-clamp-25mV.xml#simulation

Variable: ...s_buist/components/ICaL.xml#Vm

-35 mV

x-axis

Simulation: ...tage-clamp-35mV.xml#simulation

Variable: ...nts/ICa-voltage-clamp.xml#time

y-axis

Simulation: ...tage-clamp-35mV.xml#simulation

Variable: ...s_buist/components/ICaL.xml#Vm

-45 mV

x-axis

Simulation: ...tage-clamp-45mV.xml#simulation

Variable: ...nts/ICa-voltage-clamp.xml#time

y-axis

Simulation: ...tage-clamp-45mV.xml#simulation

Variable: ...s_buist/components/ICaL.xml#Vm

Done

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Resulting ICaL Current

Creator: David Nickerson (david.nickerson@nus.edu.sg) Division of Bioengineering, National University of Singapore

Created: 2007-09-11

Publisher: Division of Bioengineering, National University of Singapore

Pubmed reference: 17486452

Comment [created by David Nickerson (david.nickerson@nus.edu.sg) Division of Bioengineering, National University of Singapore]:

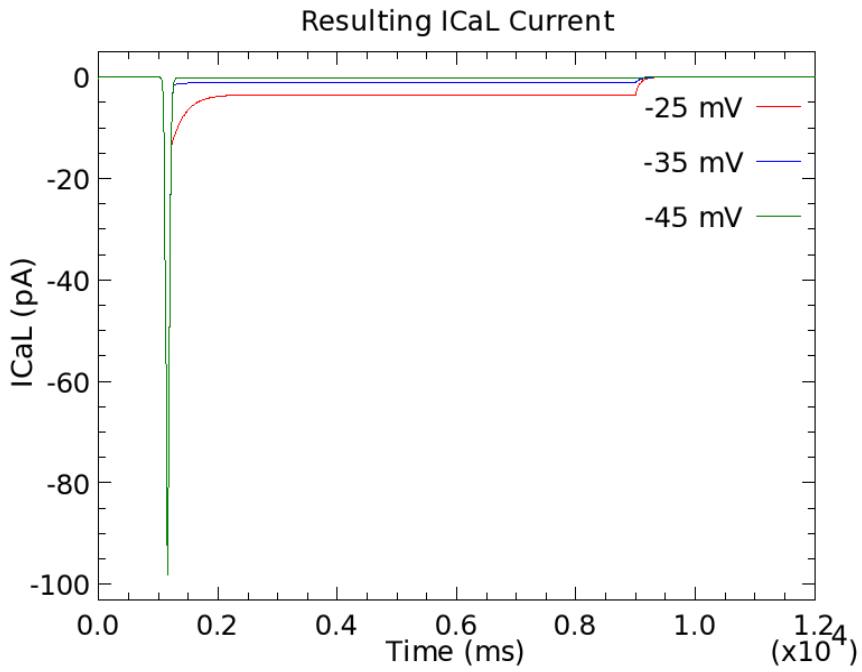
This graph partially provides a reproduction of Figure 2(D) from Corrias & Buist (2007).

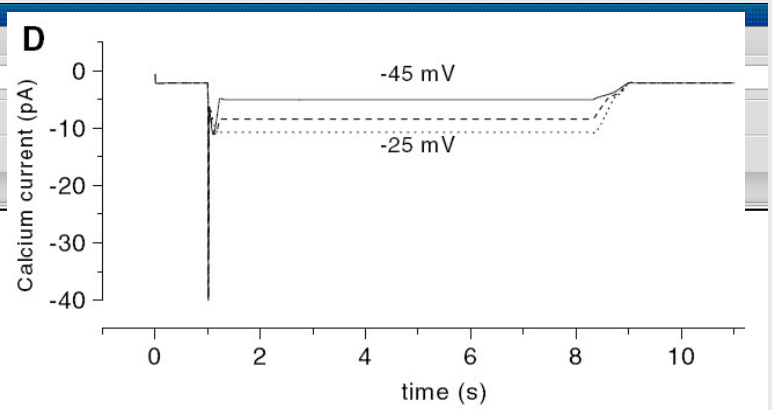
Created: 2007-11-22

Modification [modified by David Nickerson (david.nickerson@nus.edu.sg) Division of Bioengineering, National University of Singapore]:

Adding standard CellML metadata annotations to the graph descriptions.

Modified: 2007-11-22





-25 mV

x-axis

Simulation: ...tage-clamp-25mV.xml#simulation

Variable: ...nts/ICa-voltage-clamp.xml#time

y-axis

Simulation: ...tage-clamp-25mV.xml#simulation

Variable: ...buist/components/ICaL.xml#ICaL

-35 mV

x-axis

Simulation: ...tage-clamp-35mV.xml#simulation

Variable: ...nts/ICa-voltage-clamp.xml#time

y-axis

Simulation: ...tage-clamp-35mV.xml#simulation

Variable: ...buist/components/ICaL.xml#ICaL

-45 mV

x-axis

Simulation: ...tage-clamp-45mV.xml#simulation

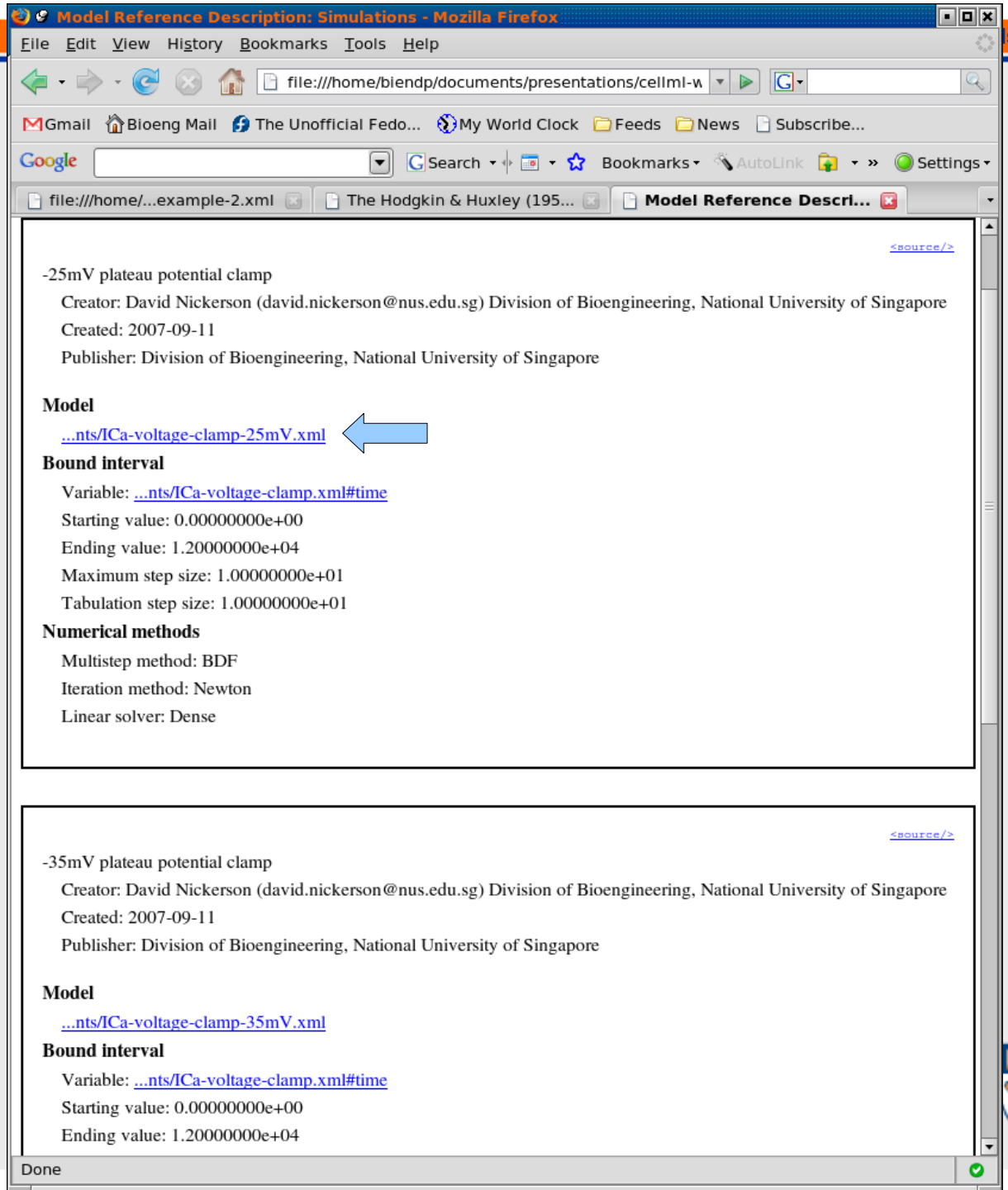
Variable: ...nts/ICa-voltage-clamp.xml#time

y-axis

Simulation: ...tage-clamp-45mV.xml#simulation

Variable: ...buist/components/ICaL.xml#ICaL

Done


Model Reference Description: Simulations - Mozilla Firefox
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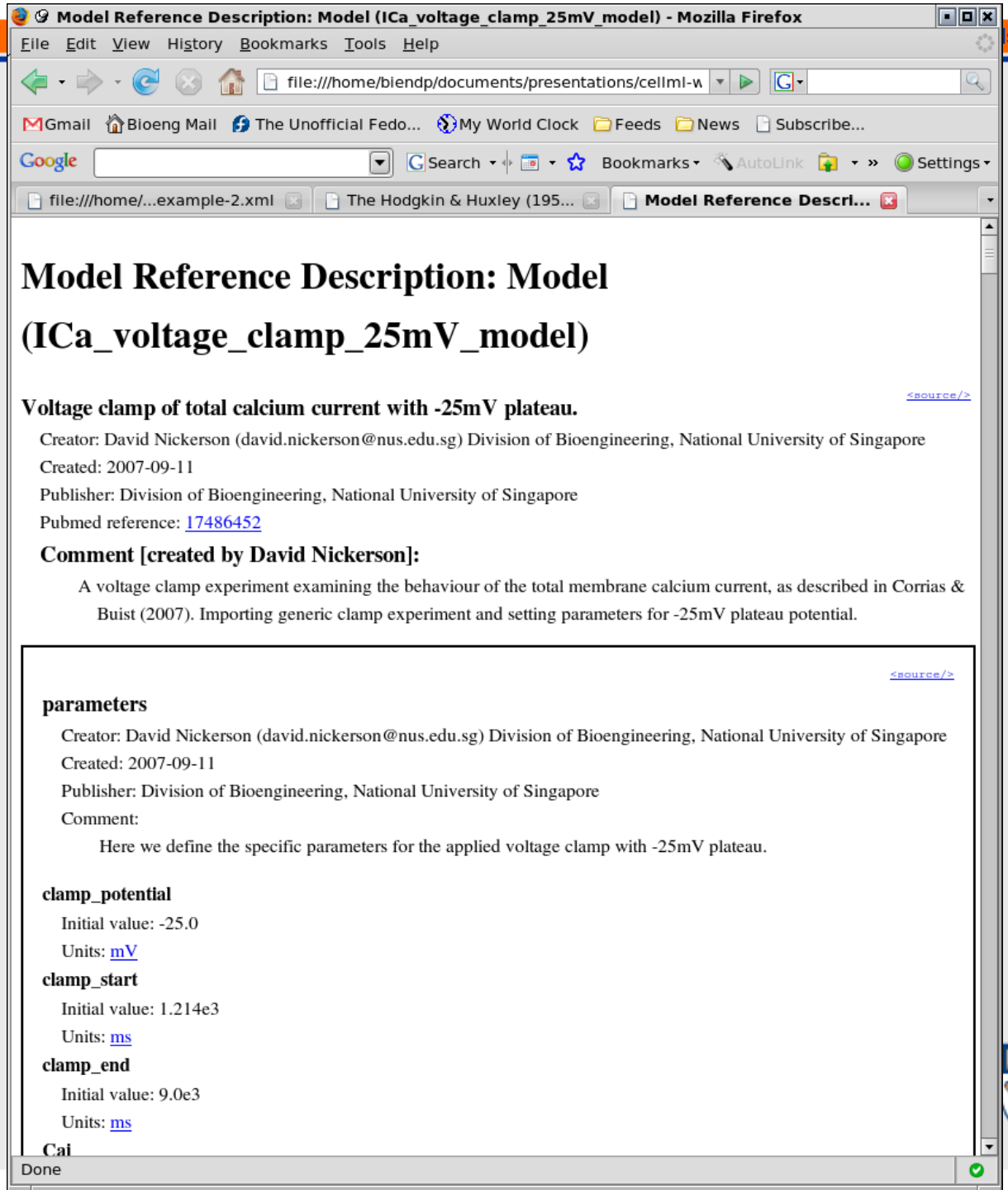
file:///home/...example-2.xml
The Hodgkin & Huxley (195...
Model Reference Descri...
<source/>
-25mV plateau potential clamp
Creator: David Nickerson (david.nickerson@nus.edu.sg) Division of Bioengineering, National University of Singapore
Created: 2007-09-11
Publisher: Division of Bioengineering, National University of Singapore
Model
...nts/ICa-voltage-clamp-25mV.xml
Bound interval
Variable: ...nts/ICa-voltage-clamp.xml#time
Starting value: 0.00000000e+00
Ending value: 1.20000000e+04
Maximum step size: 1.00000000e+01
Tabulation step size: 1.00000000e+01
Numerical methods
Multistep method: BDF
Iteration method: Newton
Linear solver: Dense
<source/>
-35mV plateau potential clamp
Creator: David Nickerson (david.nickerson@nus.edu.sg) Division of Bioengineering, National University of Singapore
Created: 2007-09-11
Publisher: Division of Bioengineering, National University of Singapore
Model
...nts/ICa-voltage-clamp-35mV.xml
Bound interval
Variable: ...nts/ICa-voltage-clamp.xml#time
Starting value: 0.00000000e+00
Ending value: 1.20000000e+04
Done



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Resulting ICaL Current

Creator: David Nickerson (david.nickerson@nus.edu.sg) Division of Bioengineering, National University of Singapore

Created: 2007-09-11

Publisher: Division of Bioengineering, National University of Singapore

Pubmed reference: 17486452

Comment [created by David Nickerson (david.nickerson@nus.edu.sg) Division of Bioengineering, National University of Singapore]:

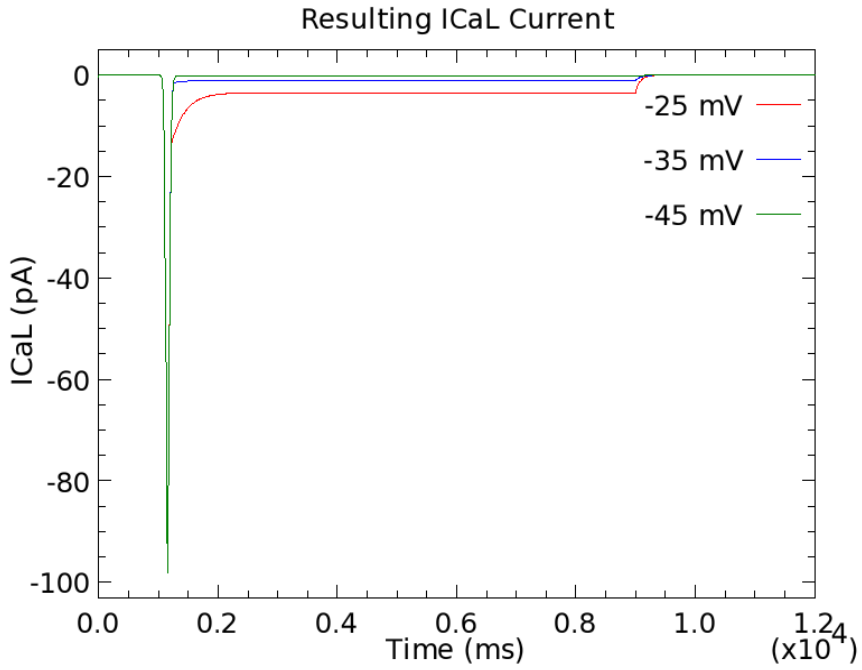
This graph partially provides a reproduction of Figure 2(D) from Corrias & Buist (2007).

Created: 2007-11-22

Modification [modified by David Nickerson (david.nickerson@nus.edu.sg) Division of Bioengineering, National University of Singapore]:

Adding standard CellML metadata annotations to the graph descriptions.

Modified: 2007-11-22



-25 mV

x-axis

Simulation: ...tage-clamp-25mV.xml#simulation

Variable: ...nts/ICa-voltage-clamp.xml#time

y-axis

Simulation: ...tage-clamp-25mV.xml#simulation

Variable: ...buist/components/ICaL.xml#ICaL

-35 mV

x-axis

Simulation: ...tage-clamp-35mV.xml#simulation

Variable: ...nts/ICa-voltage-clamp.xml#time

y-axis

Simulation: ...tage-clamp-35mV.xml#simulation

Variable: ...buist/components/ICaL.xml#ICaL

-45 mV

x-axis

Simulation: ...tage-clamp-45mV.xml#simulation

Variable: ...nts/ICa-voltage-clamp.xml#time

y-axis

Simulation: ...tage-clamp-45mV.xml#simulation

Variable: ...buist/components/ICaL.xml#ICaL

Done

Model Reference Description: Model (ICa_voltage_clamp_25mV_model) - Mozilla Firefox

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<source/>

ICaL

Creator: David Nickerson (david.nickerson@nus.edu.sg) Division of Bioengineering, National University of Singapore

Created: 2007-09-04

Publisher: Division of Bioengineering, National University of Singapore

Comment:

Here we calculate the L-type calcium current. We expect the time, membrane potential, [Ca]i, and conductance to be set externally, and we provide access to the gating variables and the calculated current. This component encapsulates all others in this model and thus acts as an interface to the gating variable components, both local and imported.

Imported as: total_Ca_current

Untitled metadata

Creator: David Nickerson (david.nickerson@nus.edu.sg) Division of Bioengineering, National University of Singapore

Created: 2007-09-10

Publisher: Division of Bioengineering, National University of Singapore

$$ICaL = g\_CaL \, d \, f \, fCa \left(Vm - ECa \right)$$

ICaL

Units: pA

g_CaL

Defined as: g_CaL

Units: nS

d

Defined as: gate

Units: dimensionless

f

Defined as: gate

Units: dimensionless

fCa

Defined as: fCa

Done

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Model Reference Description: Model (ICa_voltage_clamp_25mV_model) - Mozilla Firefox

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Units: dimensionless

Units definitions

mV

$(1000\ \text{second}^{-3})\ (\text{ampere}^{-1})\ (\text{kilogram})\ (\text{metre}^{2})$

ms

1000 second

mM

1e+09 mole $(1\text{e-}09\ \text{metre}^{-3})$

pA

1e+12 ampere

nS

$(1\text{e+}09\ \text{second}^{3})\ (\text{ampere}^{2})\ (\text{kilogram}^{-1})\ (\text{metre}^{-2})$

dimensionless

dimensionless

K

kelvin

gas_constant

$(1\text{e+}12\ \text{second}^{-2})\ (\text{kelvin}^{-1})\ (\text{kilogram})\ (1\text{e-}09\ \text{mole}^{-1})\ (\text{metre}^{2})$

faradays_constant

1e+09 second (ampere) $(1\text{e-}09\ \text{mole}^{-1})$

Created: 02:59:06 2008-03-18 (UTC) by CellMLSimulator

Done

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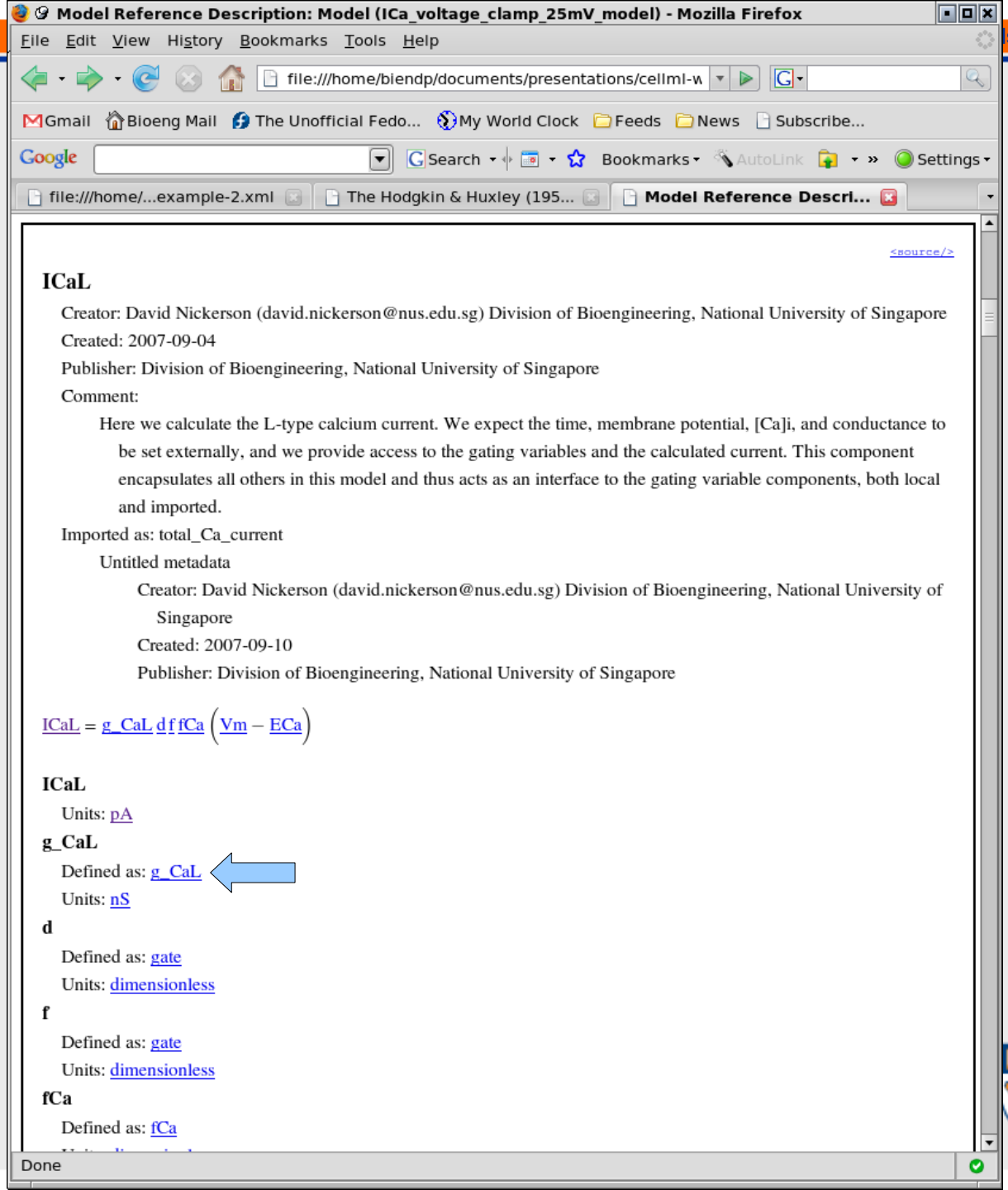

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g_CaL

Initial value: 65.0

Units: nS

Metadata

Pubmed reference: 1312782

Biological Entity: gastric smooth muscle

Species: canine

Comment:

Maximal conductance of the L-type calcium current.

d_V_half

Initial value: 17.0

Units: mV

Metadata

Pubmed reference: 7683715

Biological Entity: oesophageal muscularis mucosae

Species: New Zealand White rabbit

Comment:

Half maximal potential for voltage-dependent activation gate for L-type calcium current.

d_k

Initial value: 4.3

Units: mV

Metadata

Comment:

Slope factor for voltage dependence of L-type calcium current activation gate.

f_V_half

Initial value: 43.0

Units: mV

Metadata

Comment:

Half maximal potential for voltage-dependent inactivation gate for L-type calcium current.

f_k

Initial value: 8.9

Units: mV

Done

Model Reference Description: Model (ICa_voltage_clamp_25mV_model) - Mozilla Firefox

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<source/>

Default model parameter values

Creator: David Nickerson (david.nickerson@nus.edu.sg) Division of Bioengineering, National University of Singapore

Created: 2007-09-05

Publisher: Division of Bioengineering, National University of Singapore

Comment:

Here we define the complete set of default parameter values.

Modification [modified by David Nickerson]:

Adding parameter data for the IKA current.

Modified: 2007-11-26

Modification [modified by David Nickerson]:

Separating out the calculation of the Ca temperature correction factor.

Modified: 2007-11-26

Imported as: default_parameters

Untitled metadata

Creator: David Nickerson (david.nickerson@nus.edu.sg) Division of Bioengineering, National University of Singapore

Created: 2007-09-10

Publisher: Division of Bioengineering, National University of Singapore

$$\text{Tcorrection\_Ca} = \text{Q10Ca}^{\left(\text{T} - \text{T\_Ca} / \left[10.0\text{K}\right]\right)}$$

$$\text{Tcorrection\_K} = \text{Q10K}^{\left(\text{T} - \text{T\_K} / \left[10.0\text{K}\right]\right)}$$

$$\text{tau\_d} = \text{tau\_d\_base}\ \text{Tcorrection\_Ca}$$

$$\text{tau\_f} = \text{tau\_f\_base}\ \text{Tcorrection\_Ca}$$

$$\text{tau\_xA2} = \text{tau\_xA2\_base}\ \text{Tcorrection\_K}$$

Tcorrection_Ca

Units: dimensionless

Q10 temperature correction factor for calcium.

Q10Ca

Initial value: 2.1

Units: dimensionless

Done

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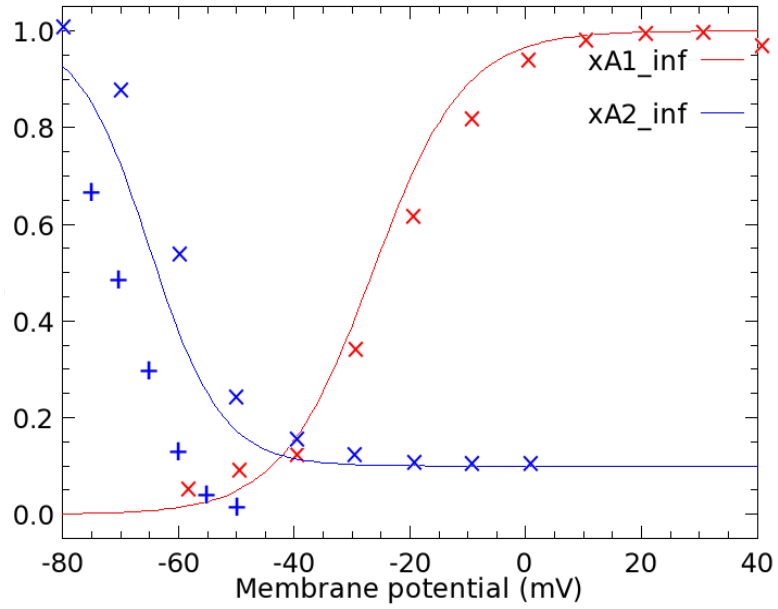


Simulation: ...A-voltage-clamp.xml#simulation
Variable: ...ments/IKA-voltage-clamp.xml#Vm

y-axis

Simulation: ...A-voltage-clamp.xml#simulation
Variable: ...ist/components/IKA.xml#xA1_inf

Experimental Data

×

IKA steady state activation gating kinetics data from Amberg et al (2002).
Creator: David Nickerson (david.nickerson@nus.edu.sg) Division of Bioengineering, National University of Singapore
Created: 2007-11-24
Pubmed reference: 12381815
Biological Entity: gastric antrum
Species: mouse
Data source: ...ate-gating-data-activation.csv [text/csv; header=present]

Comment:

Data used to fit the steady state activation gating kinetics of the IKA current in the Corrias & Buist (2007) smooth muscle cellular electrophysiology model.

Modification [modified by David Nickerson]:

Splitting the combined data into separate resources for ease of use.
Modified: 2007-11-26

xA2_inf

x-axis

Simulation: ...A-voltage-clamp.xml#simulation
Variable: ...ments/IKA-voltage-clamp.xml#Vm

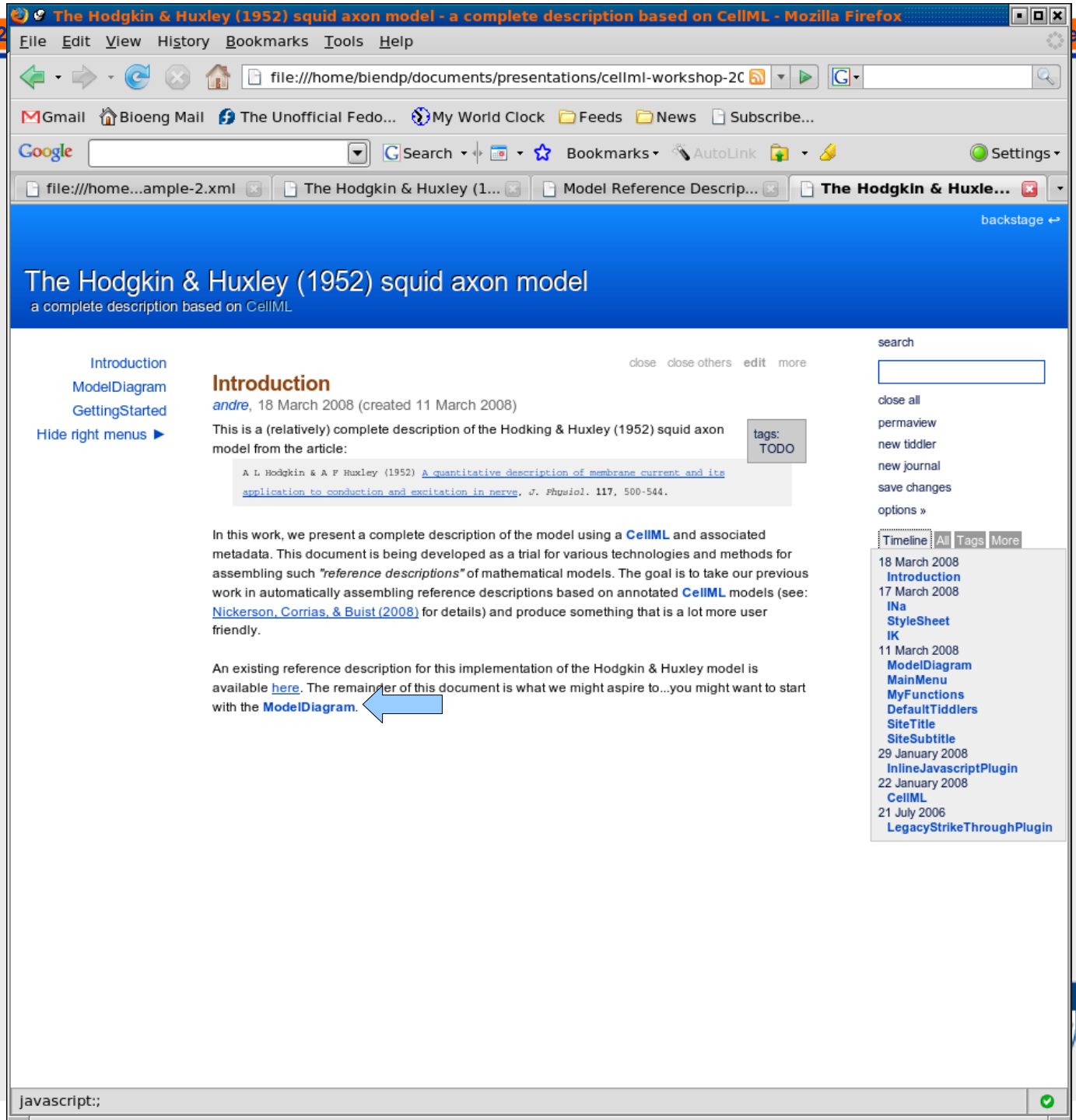
y-axis

Simulation: ...A-voltage-clamp.xml#simulation
Variable: ...ist/components/IKA.xml#xA2_inf

Experimental Data

×

IKA steady state inactivation gating kinetics data from Amberg et al (2002).
Creator: David Nickerson (david.nickerson@nus.edu.sg) Division of Bioengineering, National University of Singapore
Created: 2007-11-24
Pubmed reference: 12381815
Biological Entity: gastric antrum
Species: mouse
Data source: ...e-gating-data-inactivation.csv [text/csv; header=present]


The Hodgkin & Huxley (1952) squid axon model - a complete description based on CellML - Mozilla Firefox
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Model Reference Descrip...
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The Hodgkin & Huxley (1952) squid axon model
a complete description based on CellML
Introduction
ModelDiagram
GettingStarted
Hide right menus ▶
close close others edit more
Introduction
andre, 18 March 2008 (created 11 March 2008)
This is a (relatively) complete description of the Hodking & Huxley (1952) squid axon model from the article:
tags: TODO
A L Hodgkin & A F Huxley (1952) A quantitative description of membrane current and its application to conduction and excitation in nerve, J. Physiol. 117, 500-544.
In this work, we present a complete description of the model using a CellML and associated metadata. This document is being developed as a trial for various technologies and methods for assembling such "reference descriptions" of mathematical models. The goal is to take our previous work in automatically assembling reference descriptions based on annotated CellML models (see: Nickerson, Corrias, & Buist (2008) for details) and produce something that is a lot more user friendly.
An existing reference description for this implementation of the Hodgkin & Huxley model is available here. The remainder of this document is what we might aspire to...you might want to start with the ModelDiagram.
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close all
permaview
new tiddler
new journal
save changes
options »
Timeline All Tags More
18 March 2008
Introduction
17 March 2008
INa
StyleSheet
IK
11 March 2008
ModelDiagram
MainMenu
MyFunctions
DefaultTiddlers
SiteTitle
SiteSubtitle
29 January 2008
InlineJavascriptPlugin
22 January 2008
CellML
21 July 2006
LegacyStrikeThroughPlugin
javascript:;

The Hodgkin & Huxley (1952) squid axon model - a complete description based on CellML - Mozilla Firefox

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The Hodgkin & Huxley (1952) squid axon model

a complete description based on CellML

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Introduction

andre, 18 March 2008 (created 11 March 2008)

This is a (relatively) complete description of the Hodking & Huxley (1952) squid axon model from the article:

tags: TODO

> A L Hodgkin & A F Huxley (1952) A quantitative description of membrane current and its application to conduction and excitation in nerve. *J. Physiol.* **117**, 500-544.

In this work, we present a complete description of the model using a **CellML** and associated metadata. This document is being developed as a trial for various technologies and methods for assembling such *"reference descriptions"* of mathematical models. The goal is to take our previous work in automatically assembling reference descriptions based on annotated **CellML** models (see: Nickerson, Corrias, & Buist (2008) for details) and produce something that is a lot more user friendly.

An existing reference description for this implementation of the Hodgkin & Huxley model is available here. The remainder of this document is what we might aspire to...you might want to start with the **ModelDiagram**.

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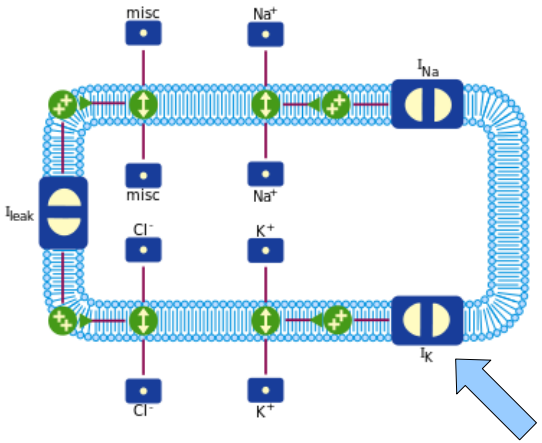
ModelDiagram

andre, 11 March 2008 (created 24 January 2008)

This is the conceptual diagram of the Hodgkin & Huxley (1952) model as it was defined in the original article. The diagram is based on Sarala's (old?) glyph set combined with some elements from Peter Villiger's SVG objects from his model repository work.

no tags



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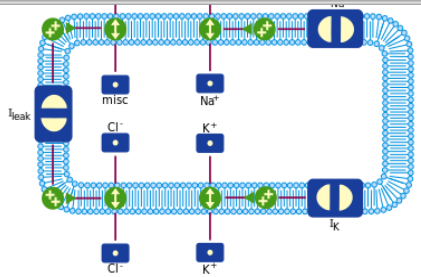
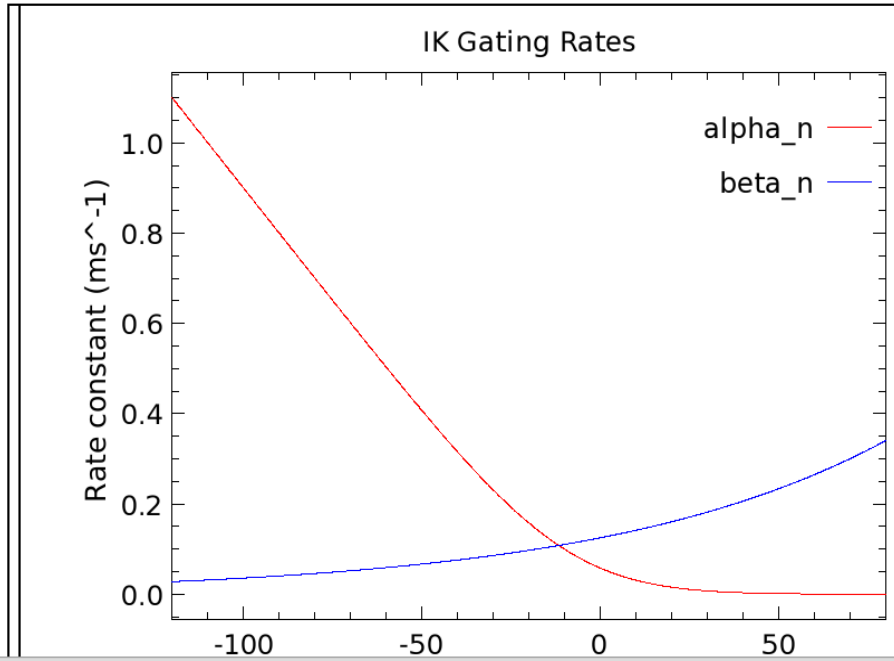


IK

andre, 17 March 2008 (created 17 March 2008)



alpha_n

x-axis

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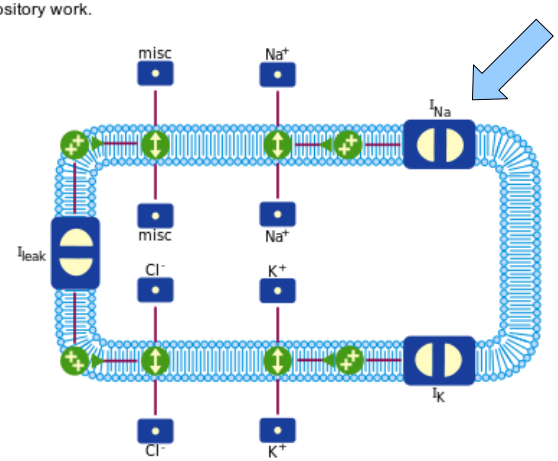

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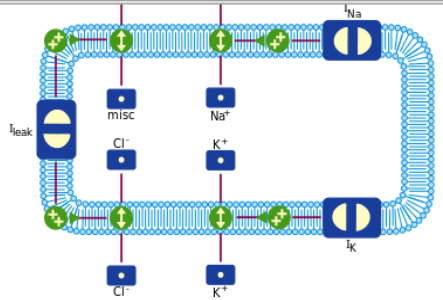
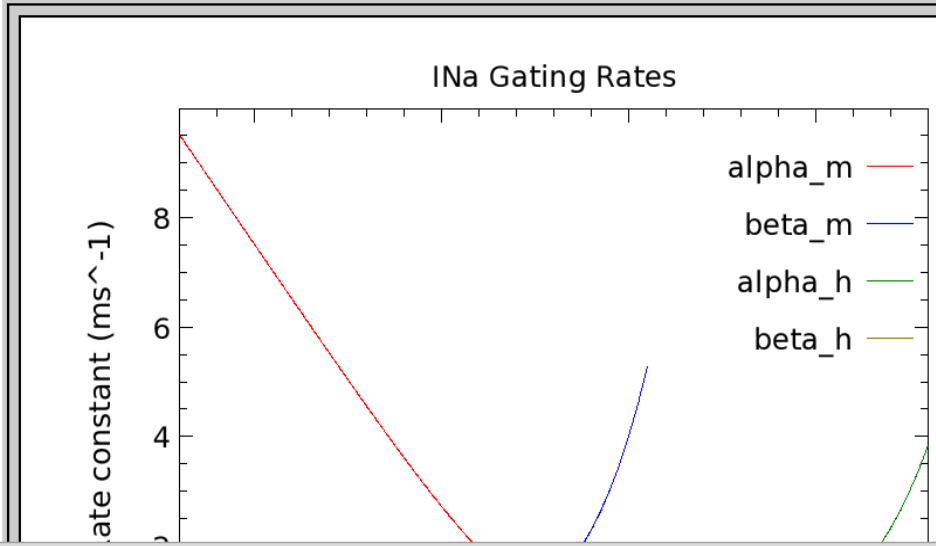


INa

andre, 17 March 2008 (created 17 March 2008)

Gating Rates	
Publisher:	Division of Bioengineering, National University of Singapore
Pubmed ID:	12991237
Species:	*loligo*
Biological entity:	giant nerve fibre



alpha_m
x-axis
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beta_m
x-axis
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alpha_h

Acknowledgments

- A*STAR BMRC Grant #05/1/21/19/383.
- Alberto Corrias.

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