#### Don't reinvent the brain Using ModelDB and other archives for your research

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Yale School of Medicine

10 November 2017

# What is ModelDB?



#### from neuron import h, rxd import neuron.rxd.node as node from matplotlib import pyplot import time

#### h.load\_file('stdrun.hoc')

soma = h.Section()
soma.L = 10
soma.diam = 10
soma.nsg = 11
dend = h.Section()
dend.connect(soma)
dend.L = 50
dend.diam = 2
dend.nseg = 51

def print\_nodes():
 print ', '.join(str(v) for v in node.\_states)

#### print 'defining rxd'

region = rxd.Region(h.allsec(), nrn\_region='i')
ca = rxd.Species(region, name='ca', d=1, charge=2, initial:
reaction = rxd.Retc(ca, -ca \* (1 - ca) \* (0.3 - ca))

print 'initializing'
h.finitialize()

print 'before:'
print\_nodes()
print

Morse TM, Carnevale NT, Mutalik PG, Migliore M, Shepherd GM (2010) Abnormal excitability of oblique dendrites implicated in early Alzheimer's: a computational study Front. Neural Circuit & (16);Methel

References and models cited by this paper

Acker CD, White JA (2007) Roles of I(A) and morphology in action potential propagation in CA1 pyramidal cell dendrities. J Comput Neurosol 23(2):201-16 [Journal] Dealed

 Roles of I(A) and morphology in AP prop. in GA1 pyramidal cell dendrites (Acker and White 2007) Model

Anderton BH, Callahan L, Coleman P, Davies P, Flood D, Joha GA, Ohm T, Weaver C (1998) Dendtilic changes in Alzheimer's disease and factors that may underlie these chances. *Proc Neurobiol* **55**:051-001 Invalued

Andrastalvy BK, Makara JK, Johnston D, Magee JC (2008) Altered synaptic and non-synaptic properties of References and models that cite this paper

Culmone V, Miglione M (2012) Progressive effect of beta amyloid peptides accumulation on CA1 pyramidal neurons: a model study suggesting possible treatments Front Constant Neurosol & Sci Journal Publied

#### CA1 pyramidal neurons: effects of Alzheimer (Culmone and Nigliore 2012) [Model]

McDougal RA, Morse TM, Hines ML, Shepherd GM (2015) ModeView for Mode/DB: online presentation of model structure Neuroinformatics 13(4):459-70 [Journal] Publied

 ModelView: online structural analysis of computational models (McDougal et al. 2015) [Model]

#### modeldb.yale.edu



# Twenty years of ModelDB and beyond: building essential modeling tools for the future of neuroscience

Robert A. McDougal<sup>1</sup> · Thomas M. Morse<sup>1</sup> · Ted Carnevale<sup>1</sup> · Luis Marenco<sup>1,2,3</sup> · Rixin Wang<sup>3,4</sup> · Michele Migliore<sup>1,5</sup> · Perry L. Miller<sup>2,3,4</sup> · Gordon M. Shepherd<sup>1</sup> · Michael L. Hines<sup>1</sup>

Received: 9 June 2016 / Revised: 17 August 2016 / Accepted: 30 August 2016 © Springer Science+Business Media New York 2016

Abstract Neuron modeling may be said to have originated with the Hodgkin and Huxley action potential model in 1952 and Rall's models of integrative activity of dendrites in 1964. groups (Allen Brain Institute, EU Human Brain Project, etc.) are emerging that collect data across multiple scales and integrate that data into many complex models, presenting new

# What is in ModelDB?

Models for:

- 178 cell types
- 16+ species
- 54 ion channels, pumps, etc
- 145 topics (Alzheimer's, STDP, etc)
- 24+ mammalian brain regions

1211 published models from 76 simulators

- 575 NEURON models
- 340 "realistic" networks
- 48 connectionist networks



Numbers are as of May 20, 2017

# Why use ModelDB?

"Non-reproducible single occurrences are of no significance to science."

- Karl Popper in The logic of scientific discovery, 1959.

#### What is needed for a model to be reproducible?

#### Model

- an approximation of the system of interest
  - e.g. a model organism or a complete statement of the properties of the model in mathematical or computable form

#### **Experimental protocol**

• what was done with the model to produce the data

Science builds upon previous work; in order to do that, the previous work needs to be reproducible.

#### Models are complicated



- 38.5% of ModelDB models have over 20 files; 24.2% of files are over 5K.
- It is often hard to fully describe this complexity in a paper.
- Any bugs, typos, errors, or omissions might completely change the dynamics.

Distributions from ModelDB, Fall 2013. A model was counted as having 0 files if it was not hosted on ModelDB.

The easiest way to replicate someone else's results – a first step toward building on them – is to get their model code from a repository such as ModelDB.

But beware:

- They may be solving a different problem than you (with respect to species, temperature, age, etc).
- Their code may have bugs.

To reduce the risk of problems:

- Read the associated paper.
- **Compare** the model and results to other similar models.
- **Examine** the model with ModelView and/or psection.
- **Test** ion channels individually.
- Collaborate with an experimentalist.

# Reproducibility in Computational Neuroscience Models and Simulations

Robert A. McDougal, Anna S. Bulanova, William W. Lytton

Abstract—Objective: Like all scientific research, computational neuroscience research must be reproducible. Big data science, including simulation research, cannot depend exclusively on journal articles as the method to provide the sharing and transparency required for reproducibility. build novel theoretical frameworks. A century ago, work by Lapicque led to the development of integrate-and-fire models [4]. A half century later, Hodgkin and Huxley provided a detailed multiscale biophysical model of the squid axon [2],

- Simulators (NEURON, MCell, XPPAUT, NEST, etc)
- Multi-simulator interoperability (NeuroML, SWC, PyNN, NeuroConstruct, etc)
- Shared resources (Neuroscience Gateway, Simulation Platform)
- Sharing resources (ModelDB, OpenSourceBrain, NeuroMorpho.Org, etc)
- More: NSDF, NeuroLex, NIF, MIASE, licensing, etc

McDougal et al (2016) IEEE TBME 63(10):2021-2035; doi:10.1109/TBME.2016.2539602

### Neurobiological context

#### Morphology



#### Metadata

cell types, channels, receptors, genes, transmitters, model topics, publication

#### NeuronDB

Overview Data/Search pl	us Connectivity	pha Gausical References/Notes	Hodels	BrainPharm
	Hippocamp.	is CA1 pyramidal cell		
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# Model Entry Amyloid beta (IA block) effects on a model CA1 pyramidal cell (Morse et al. 2010)

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implementar(s);	Community, Tart (Text, Communite at Yole, anti-); Minner, Tom (Committenes at Yole, anti-);

#### Microconnectome



#### Electrophysiology



ModelDB is a place to see what has been modeled in a cell type.

Not only can you get code, but by comparing models, you can see what mechanisms are considered critical by the community.



### How to use ModelDB

# Finding models

hin	Q		
hinf			
hinf-h			
hines			
hinton.hoc			
hint			
Authors			
Hines ML		>	View all
Hines M		>	
Cell Type			Olfactory Mitral Cell (Shen et al 1999)
Entorhinal cortex stellate	e cell		Arteriolar networks: Spread of potential (Crane et al 2001)
Region			Olfactory Mitral cell: AP initiation modes (Chen et al 2002)
Entorhinal cortex			Local variable time step method (Lytton, Hines 2005)
Transmitter			Olfactory bulb mitral cell: synchronization by gap junctions
Norephinephrine			(Migliore et al 2005)
Ephinephrine			Discrete event simulation in the NEURON environment (Hines
Dynorphin			and Carnevale 2004)
Receptor			Spatial gridding and temporal accuracy in NEURON (Hines and
Dynorphin			Carnevale 2001)
Concept			•
Tutorial/Teaching			

- Search box on the top-left of every page.
- Do full text or attribute searches.
- Word completions (based on ModelDB entries not English) and attribute results updated as you type.
- Advanced search and browsing are also available.

### ShowModel features



(1) Search models. (2) Browse models. (3) Link to download the entire model code.
 (4) Auto-launch a NEURON simulation (requires browser configuration). (5) View model files.
 (6) Find models and papers cited by this model's paper, or that cite this model. (7) ModelView: visualize model structure. (8) Simulation platform (5 minutes of remote desktop access to experiment with the model). (9) 3D printable versions of cells from the model (in 3DModelDB).
 (10) Description of model. (11) Paper(s) describing or using model. (12) Searchable metadata.
 (13) Links to NeuronDB (channel distributions etc within cell types).

#### Amyloid beta (IA block) effects on a model CA1 pyramidal cell (Morse et al. 2010)

		Download	zip file Auto-launch	1					
Help downloading and running models									
Model Information	Iodel File Citations	Model Views	Simulation Platform	* 3D Print					
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(14) Download the currently selected file. (15) Directory browser, showing model files.(16) View pane for the currently selected file.

# Identifying existing reuse

#### Amyloid beta (IA block) effects on a model CA1 pyramidal cell (Morse et al. 2010)



Asterisks in the file browser indicate that the file is reused in other models; click the asterisk to see a list of the other models.

## ICGenealogy: ion channel metadata

Model Information Model File	Citations	Model Views	Simulation Platform	* 3D Print
Download the displayed file [ICGeneal	ogy			
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#### General data

- ICG id: 2464
- ModelDB id: 87284
- Reference: Morse TM, Carnevale NT, Mutalik PG, Migliore M, Shepherd GM (2010): Abnormal Excitability of Oblique Dendrites Implicated in Early Alzheimer's: A Computational Study.

#### Metadata classes

- Animal Model: rat
- Brain Area: hippocampus, CA1
- Classes: KCa
- Ion Type: K
- Neuron Region: unspecified
- Neuron Type: pyramidal cell
- Runtime Q: Q4 (slow)
- Subtype: not specified

#### Metadata generic

- Age: 7-14 weeks old.
- Comments: Calcium activated k channel, modified from moczydlowski and latorre (1983). From hemond et al. (2008), model no. 101629, with no changes (identical mod file). Animal model taken from chen (2005) which is used to constrain model. Channel kinetics from previous study on hippocampal pyramidal neuron (hemond et al. 2008)
- Runtime: 76.722

When viewing most mod files describing an ion channel, an ICGenealogy button appears. Clicking this button loads the corresponding page of the ICGenealogy database which shows curated information about the channel model (how it was derived, information about the underlying data, etc) and response curves.

Podlaski, Seeholzer, Vogels

#### Amyloid beta (IA block) effects on a model CA1 pyramidal cell (Morse et al. 2010)

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The model simulations provide evidence oblique dendrites in CA1 pyramidal neurons are susceptible to hyper-excitability by amyloid beta block of the transient K+ hannel, IA. See paper for details. <b>Reference:</b> 1. Morse TM, Carnevale NT, Mutalik PG, Migliore M, Shepherd GM (2010) Abnormal excitability of oblique dendrites implicated in early Alzheimer's: a computational study <i>Front. Neural Circuits</i> 4:16 [PubMed]									
Model Information (Click	on a link to fi	nd other models	with that proper	ty)					
Model Ty	pe: Neuron o	r other electrica	lly excitable cell;						
Brain Region(s)/Organis	sm:								
Cell Type	(s): Hippocan	npus CA1 pyran	nidal cell;						
Channel	(s): INa,t; IL	high threshold;	I N; I T low thres	hold; I A; I K	(; I h;				
Gap Junctic	ns:								
Receptor	(s):								
Gene	(s):								
Transmitter	(s):								
Simulation Environme	ent: NEURON	l;							
Model Concept	(s): Dendritic	Action Potential	ls; Active Dendrit	es; Detailed	Neuronal Mod	els; Pathophys	siology; Aging/Alzheimer`s	6	
Implementer	(s): Carneval	e, Ted [Ted.Carr	nevale at Yale.ed	u]; Morse, T	om [Tom.Morse	e at Yale.edu];			
Search NeuronDB for in	ormation abou	it: Hippocampu	is CA1 pyramidal	cell; I Na,t;	I L high thresho	old; I N; I T low	/ threshold; I A; I K; I h;		







na3









#### How do people use ModelDB?

- Find a model described in a paper, download it, and experiment to understand the model's predictions.
- Find a model described in a paper. Use ModelView to understand the model's structure.
- Locate models and modeling papers on a given topic.
- Locate model components (e.g. L-type calcium channel) for potential reuse.
- Search for simulator keywords (e.g. FInitializeHandler) to find examples of how to use them.

You can help by sharing your model code on ModelDB after publication.

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Advanced search	SenseLab		ModelDB	<b>小米</b> X前日	SimToolDB
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Find models of	
Realistic Networks	You may Subma with just the above information, but to make your model more discoverable, please fill out as much of the next section as you can. Note:
Neurons	Your model will remain private until you request the ModelDB administrator make it public.
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Neurons Electrical synapses (gap junctions) Chemical synapses Ion channels	Let us find ModelDB keywords for you!
Neuromuscular junctions Axons	Click the button to automatically find, approve, and populate model entry keywords based on your paper abstract.
Other resources	
ModelDB related resources	Additional information
Computational neuroscience	Additional Information: More information will help your model more discoverable
ecosystem	Model Name

McDougal, Dalal, Shepherd in preparation; abstract from Morse et al, 2010.





### @SenseLabProject: newly available models



### Other resources

# NeuroMorpho.Org



- NeuroMorpho.Org is home to 70,025 reconstructed neurons (and glia) from 400 cell types and 41 species as of November 9, 2017.
- Warning: not every morphology was reconstructed with the intent of being in a simulation. Before using: rotate to check for *z*-axis errors, check to make sure the diameters are not all equal.
- Use the Import 3D tool to import morphologies into NEURON. For details, see: neuron.yale.edu/neuron/docs/import3d

# Channelpedia (Channelpedia.epfl.ch)



Acc No	Sequence	Leigth	Source
NM_013119			NOBI
NM_018732			NON

#### Models

#### [1] Nav1.3 (Model ID = 43)

Animal	nat	
CellType	Neocortical	
Age	0 Deys	1.10-1
Temperature	23.0°C	
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mpower	3.0	
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htef	1 /(1+0xp([v-(-65.0))/8.1))	
nTea .	0.40 + (0.265 * exp(-x/9.47))	



[41] Thirwinaparya R. et al. Distribution and functional characterization of human New J 3 splice variantis. Eur. J. Resness, 2008 Sci., 22 (1-9).

[G] Tan 1 of all shares and not have 1.1 voltage-gated codesn channels differ in inactivation properties and constitutly to the pyredwood insecticide influence

- Home to information about ion channels.
- Many channels have one or more associated models (e.g. different species or cell types); all are downloadable as MOD files.
- Shows gating variable and channel response to voltage clamp for each model.

# Biomodels (www.ebi.ac.uk/biomodels-main)

EMBL-EBI 🌘									Services	Research Tra	ining About us
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Model	Overview	Math	Physical entities	Parameters	Cutation						
				Refe	rence Publication						
Publication ID: 12775757		Leloup JC, Goldbeter A. Toward a detailed computatio Proc. Natl. Acad. Sci. U.S.A. Unité de Chronobiologie Théo	nal model for the mammalian 2003 Jun; 100(12): 7051-705 rique, Faculté des Sciences,	n circadian clock. 6 , Université Libre de Bruxelle	rs, Campus Plaine, C. P. 2	31, B-1050 Brussels, Beig	ium. <u>Imarel</u>				
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- Biomodels is a systems biology model repository.
- Models are in SBML but can be converted to MOD files via e.g. jNeuroML (github.com/NeuroML/jNeuroML). Test converted models before using in a larger model. Edits will likely be necessary to get them to interoperate with other mechanisms.
- A native SBML importer for NEURON's rxd module is under development.

# Open Source Brain (OpenSourceBrain.org)



- Open Source Brain promotes collaborative model development via github.
- Models are typically in NeuroML or neuroConstruct format; neuroConstruct (neuroConstruct.org) converts both formats to NEURON.
- The conversion process places different ion channels in different MOD files, which allows extracting model components.

# NeuroElectro (NeuroElectro.org)



- NeuroElectro archives experimentally measured electrophysiology values for different cell types; it shows the spread and allows comparing values across different cell types.
- Read the paper associated with a value to understand: species, experimental conditions, etc.

# SenseLab (senselab.med.yale.edu)

ModelDB	NeuronDB	
NeuronDB	Back Overview Data/Search plus Connectivity plus Classical References/Notes Models BrainPharm	Julie User Public
MicroeireuitDE	Hippocampus CA1 pyramidal cell	
3DModelDB	Ave: Present Absent Neuron Type: principal Organizations Vertekarans	
	ElectroPhysiology: <u>NeuroElectro.cg</u> Pharmacology: <u>ULPIAR</u> Reconstructions: <u>MeuroMatho.Org</u>	
OlderMapDB	Genes: <u>Allen Brah Alas - Links</u> Genes: <u>Human Brah Transcriptome</u> NeuroLex:	
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dorDB	Distal apical dendrite Hacocampus CAL oriens alveus interneuron Axon terminal Galas AMPA A MPA A MPA A MPA A M A M A M A M	1 N
BBHodelDB	Perforant pathway enformal pyramoal neuron terminals (T) <u>Silutamate II. high threshold</u> Loa Lb	Locations of
BrainPharm	Middle apicat dendrite Hippocampus CA1 offens alvus interneuron Axon formial Gaba GabaA I Na.1 Hippocampus CA2 offens alvus interneuron Axon formial Gaba GabaB Caba Hippocampus CA3 pyramidal cell Axon terminal, Glutamate NMDA LPotassium	Pyramidal

- SenseLab is a suite of 10 interconnected databases (listed at left).
- ModelDB and NeuronDB (at right) are the most useful for modeling.
- NeuronDB shows what channels are present and the inputs and outputs by cell region (e.g. distal apical dendrite vs proximal apical dendrite).

#### Twitter

Many groups announce new developments on Twitter, including:

- SenseLab (including ModelDB): @SenseLabProject
- Open Source Brain: @OSBTeam
- NeuroMorpho.Org: @NeuroMorphoOrg
- ICGenealogy Project: @ICGenealogy
- Int. Neuroinformatics Coordinating Facility (INCF): @INCForg