#### Don't reinvent the brain

Using ModelDB and other archives for your research

Robert A. McDougal

Yale School of Medicine

16 October 2015

General issues •000

General issues

#### On reproducibility

"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

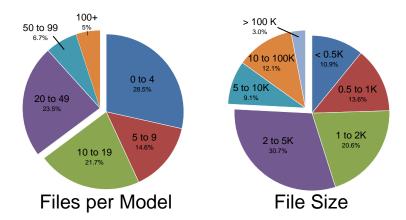
 an approximation of the system of interest
 e.g. a model organism or a complete statement of the properties of the model in mathematical or computable form

#### **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.

# Model sharing helps, but only reuse what you understand

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.

## ModelDB

Part of the SenseLab Project

 General issues
 ModelDB
 Other resources
 Stay up to date

 0000
 0 ●000000000
 0000000
 0





SimToolDB

ModelDB Help User account Login

Register Find models by

Model name First author

Each aut

Region(circuits)

Find models for

Cell type

Receptor

Transmitte

Topic

Simulators

Find models of

Networks

Neurons Electrical synapses (gap

junctions) Chemical synapses

lon channels

Neuromuscular junctions

Axons

Other resources
ModelDB related resources

Models in mercurial repository ModeIDB provides an accessible location for storing and efficiently retrieving computational neuroscience models. ModeIDB is tightly coupled with NeuronDB. Models can be coded in any language for any environment. Model code can be viewed before downloading and browsers can be set to auto-launch the models. For further information, see model sharing in general and ModeIDB in particular.

#### Search

Use the "search" box in the upper left corner to find model entries

by accession number

- by a particular author
- by keyword (cell type, region, receptor, gene, transmitter, topic, simulator)
- use advanced search for ion currents: because these are short they are problematic to search with free text
- use advanced search for a combined keyword and full text search
   prefix case sensitive words with ^
- use \* for completions

Or you may search for publications indexed in ModelDB or PubMed.

#### New Model

Submit a new model entry

Midney to be stated

©GenseLatProject

ModeIDB Home: SerineLath Home: Helpt Questions, conversels, problems? Ernall the MidshiDB Administration How to cite ModeIDB. ModeIDB Credits. © This site in Copyright 2015 Shephert Lab. Yalls University.





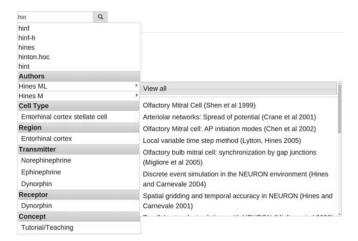
#### Models for:

- 176 cell types
- 19+ species
- 52 ion channels, pumps, etc.
- 129 topics (Alzheimer's, STDP, etc)

1052 published models from 70+ simulators

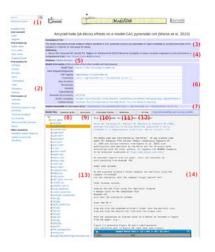
509 NEURON models

## Finding models



- 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.

## Anatomy of a ShowModel page



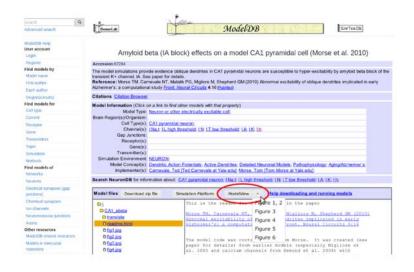
- (1) Search models.
- 2) Browse models.
- Description of model.
- (4) Paper(s) describing or using model.
- Find models and papers cited by this model's paper, or that cite this model.
- Searchable metadata.
- Links to NeuronDB (channel distributions etc within cell types).
- (8) Link to download the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

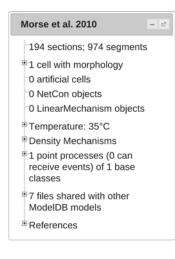
# Identifying existing reuse

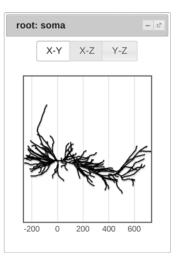


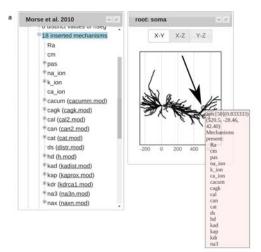
Asterisks in the file browser indicate that the file is reused in other models; click the asterisk to see a list of the other models.

#### ModelView

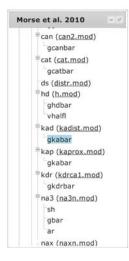


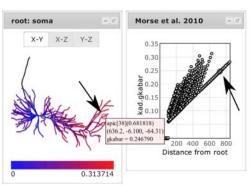
















#### How do people use ModelDB?

- 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. FlnitializeHandler) to find examples of how to use them.

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

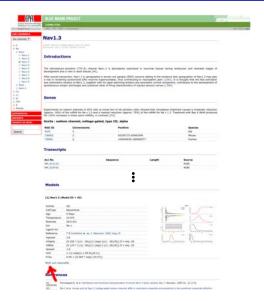
# Other resources

## NeuroMorpho.Org



- NeuroMorpho.Org is home to 31,982 reconstructed neurons from 140 cell types and 24 species as of September 24, 2015.
- 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)



- 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)



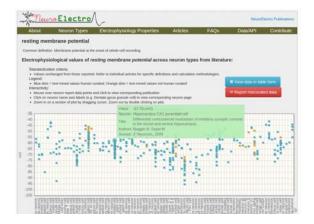
- Biomodels is a systems biology model repository.
- Models are in SBML but can be converted to MOD files via e.g.
  jNeuroML (github.com/NeuroML/jNeuroML). Test converted
  models before using in a larger model. Edits will likely be necessary
  to get them to interoperate with other mechanisms.
- A native SBML importer for NEURON's rxd module is under development.

# Open Source Brain (OpenSourceBrain.org)



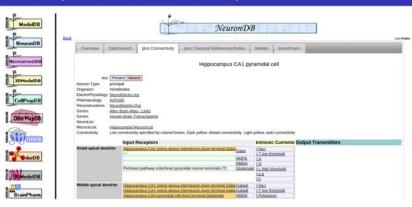
- Open Source Brain promotes collaborative model development via github.
- Models are typically in NeuroML or neuroConstruct format; neuroConstruct (neuroConstruct.org) converts both formats to NEURON.
- The conversion process places different ion channels in different MOD files, which allows extracting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



- 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).

# Stay up to date

#### Twitter

Many repositories announce new developments on Twitter, including:

- SenseLab (including ModelDB): @SenseLabProject
- Open Source Brain: @OSBTeam
- NeuroMorpho.Org: @NeuroMorphoOrg