

SciUnit

Unit Tests for
Scientific Models

Richard C Gerkin, PhD
Arizona State University, USA

Q: Why make models?

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A1: To explain and predict
the natural world.

A2:

What I cannot create,
I do not understand.

I know how to solve every
problem that has been solved

Why const & sort etc

TO LEARN:

Bethe Ansatz Probs.

Kondo

2-D Hall

local Temp

Non linear classical Hydro

$$\textcircled{A} f = u(r, \alpha)$$

$$g = \psi(r, z) u(r, z)$$

$$\textcircled{B} f = 1/r \cdot \alpha |u| u$$

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 - It is *consistent with* a wide range of previously gathered data.

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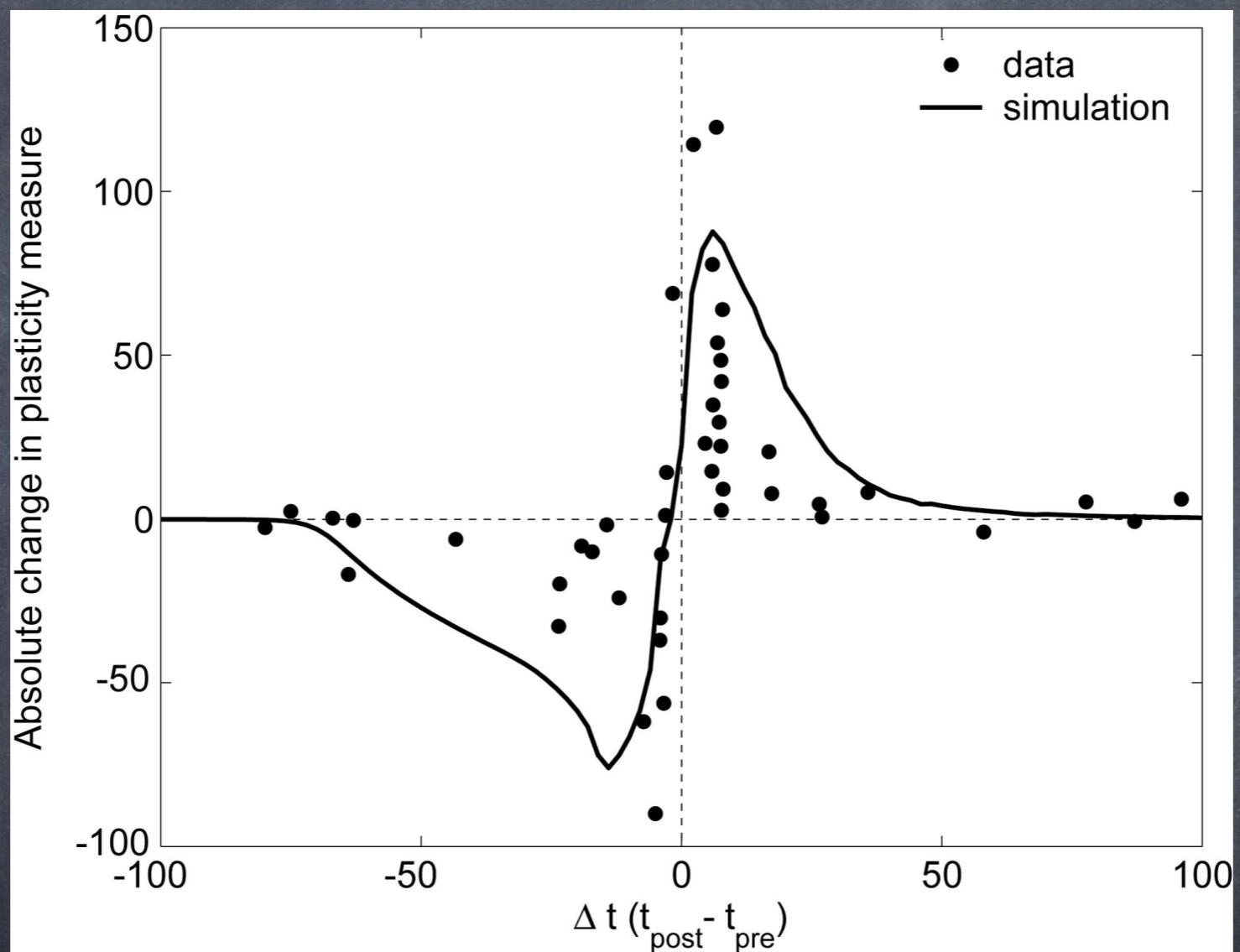
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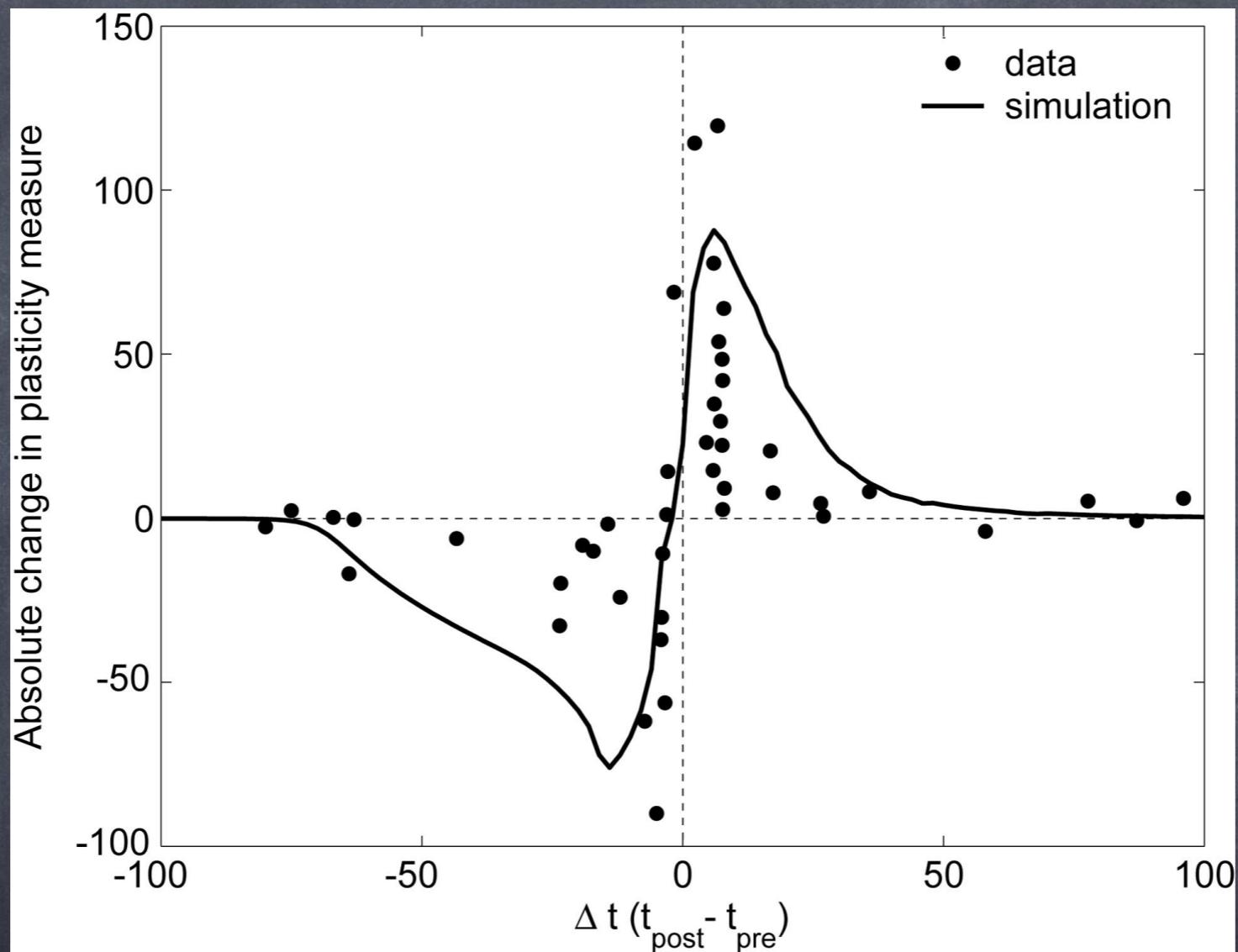
- A scientific model has high *validity* if:
 - It is *consistent with* a wide range of previously gathered data.
 - It can *predict* the results of many future experiments.

TESTING VALIDITY

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Typically, we make only *informal* arguments about a model's explanatory power.

TESTING VALIDITY



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And there is a **huge** amount of data out there now.
Informal validation is becoming increasingly difficult!

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 - What needs explaining.
- Needed: a **framework** for validating scientific models, based on established techniques for **formally validating** software.

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- $[b_{\text{low}}, b_{\text{high}}]$ are the *passing criteria*.

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- Example: A *complete* model of a cerebellar Purkinje cell should produce spikes that, given a specified description of the stimulus, **match physiologically observed** shapes, rates, interval distributions, etc.

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- <http://github.com/scidash/sciunit>

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- How to *minimize development time* for writing model validation tests?
- How to adjudicate whether a test *score* really captures the functionality it claims to test?



python™

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A: Enumerate the *capabilities* of models.

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- Each ***model*** declares its capabilities via inheritance, and satisfies them via implementation.
- Each ***test*** lists its *required capabilities*.

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Model2

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Test

Let's dance!

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Do what you said you could do with
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Model2

I can! I just forgot to
implement it. Give me a minute.

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OK, I'm ready, hit me up again.

SCIUNIT: CAPABILITIES

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OK, here are those observations again.
I'm calling your methods now.

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Test

Thanks, hold on ... hmm, your
prediction needs serious work.

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class ProducesSpikes(Capability):  
    """  
    Indicates that the model produces spikes.  
    No duration is required for these spikes.  
    """  
  
    def get_spikes(self):  
        """Gets computed spike times from the model.  
  
        Arguments: None.  
        Returns: a NeuroTools SpikeTrain object.  
        """  
  
        raise NotImplementedError()
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- Every capability is designed by a *community* of modelers and testers.
- Capabilities are *implemented* by those who understand the model being tested.

SCIUNIT: MODELS

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```
class LIFModel(sciunit.Model,ProducesMembranePotential,ProducesSpikes):
    """A leaky integrate and fire model."""

    def get_spikes(self):
        # Get membrane potential.
        membrane_potential = self.get_membrane_potential()
        # Extract spike times.
        spike_times = membrane_potential.threshold(0)
        return spike_times

    def get_membrane_potential(self):
        # Create membrane potential object from model attribute.
        membrane_potential = AnalogSignal(self.v_m, self.dt)
        return membrane_potential

    def simulate(self, ...):
        # Sets v_m, etc.
        ...
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- *SciUnit* models declare their capabilities via *inheritance*.
- *SciUnit* models *implement* capabilities to match the design of the underlying real model.

SCIUNIT: CAPABILITIES

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class ProducesActionPotentials(ProducesSpikes):  
    """Indicates the model produces action potential waveforms.  
    Waveforms must have a temporal extent.  
    """  
  
    def get_action_potentials(self):  
        """Gets action potential waveform chunks from the model.  
  
        Returns  
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        NeuroTools.signals.AnalogSignalList  
            A list of spike waveforms  
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- Previously unconsidered capabilities can be added easily.

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    def get_action_potential_widths(self):  
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- Auxiliary methods (relying on the core methods) are available to accelerate the workflow.

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- Tests are inherently **subjective**.

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```
class SpikeWidthTest(sciunit.Test):
    """Tests the full widths of spikes at their half-maximum."""

    def __init__(self,
                 observation={'mean':None,'std':None},
                 name="Action potential width"):
        """Takes the mean and standard deviation of observed spike widths"""

        Test.__init__(self,observation,name)

    required_capabilities = (ProducesMembranePotential,ProducesSpikes,)

    description = "A test of the widths of action potentials \
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    score_type = sciunit.scores.ZScore

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 - What kind of score it will return.

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    def validate_observation(self, observation):
        try:
            assert type(observation['mean']) is float
            assert type(observation['std']) is float
        except Exception,e:
            raise ObservationError("Observation must be of the form \
                {'mean':float,'std':float}")
    def generate_prediction(self, model):
        """Implementation of sciunit.Test.generate_prediction."""
        # Method implementation guaranteed by ProducesSpikes capability.
        widths = model.get_spike_widths()
        # Put prediction in a form that compute_score() can use.
        prediction = {'mean':np.mean(widths),
                      'std':np.std(widths)}
        return prediction
    def compute_score(self, observation, prediction):
        """Implementation of sciunit.Test.score_prediction."""
        score = sciunit.utils.analysis.zscore(observation,prediction)
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- The *sciunit.Test* base class has a *judge* method which takes a model, checks capabilities, and invokes all of the above to return a score.

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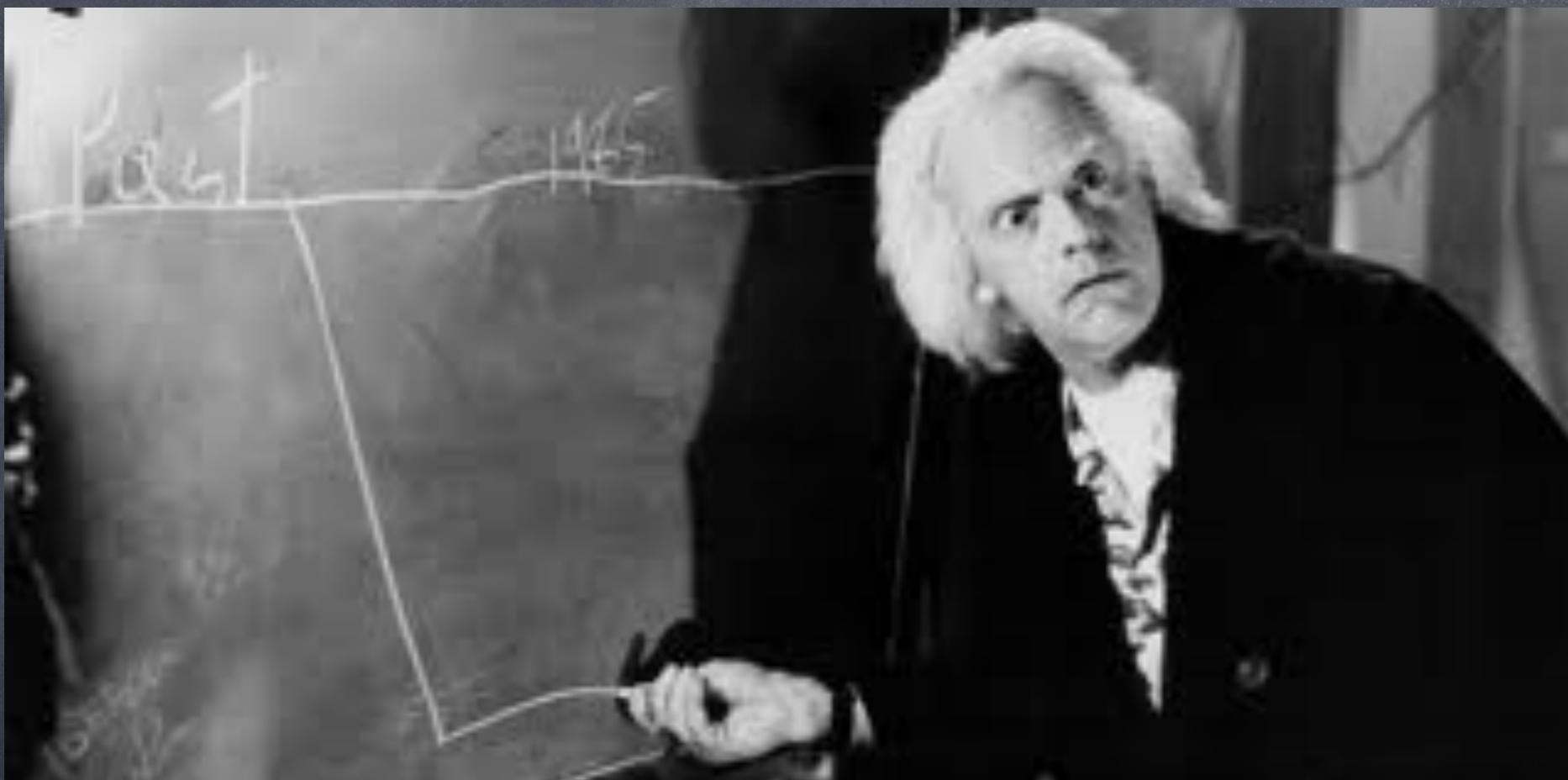
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Fork it!



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```
class InjectedCurrentSpikeWidthTest(SpikeWidthTest):  
    """Tests the full widths of spikes at their half-maximum under current injection."""  
  
    def __init__(self,  
                 observation={'mean':None,'std':None},  
                 name="Action potential width under current injection",  
                 params={'injected_current':{'ampl':0.0}}):  
        """Takes a steady-state current to be injected into a cell."""  
  
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    ...
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```
def injection_params(amplitude):  
    return {'injected_current':{'ampl':amplitude}}:  
  
width_test_1 = InjectedCurrentSpikeWidthTest(observation, injection_params(25.0))  
width_test_2 = InjectedCurrentSpikeWidthTest(observation, injection_params(50.0))  
width_test_3 = InjectedCurrentSpikeWidthTest(observation, injection_params(75.0))  
  
width_suite = sciunit.TestSuite([width_test_1,width_test_2,width_test_3])
```

SCIUNIT: WORKFLOW

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```
from QSNMC.tests import tests
from QSNMC.models import models

for model in models:
    for test in tests:
        score = test.judge(model)
        score.summarize()
```

VISUALIZING VALIDITY

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Prediction Method	19	20	21	22	RMS
Ohl's method	-55.4	19.1	21.8	4.4	31.3
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TestSuite([SunspotTest(cycle_data) for cycle_data in all_cycle_data])
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- Everyone immediately sees where it stands with respect to all previously test-encoded data!

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- When new experimental data is produced, we add a new column.

VISUALIZING VALIDITY

```
TestSuite([SunspotTest(cycle_data) for cycle_data in all_cycle_data])  
.judge([OhlsMethod, FeynmansMethod, ThompsonsMethod]).view()
```

Model	SunspotTest(19)	SunspotTest(20)	SunspotTest(21)	SunspotTest(22)
OhlsMethod	-55.4	19.1	21.8	4.4
FeynmansMethod	-42.8	9.6	26.9	3.6
ThompsonsonMethod	-17.8	8.7	-26.5	-13.6

- When new experimental data is produced, we add a new column.
- Everyone immediately sees how valid all existing models are against it!

COMPETITION

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from QSNMC.tests import tests
from QSNMC.models import models

for model in models:
    for test in tests:
        score = test.judge(model)
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<https://github.com/incf/qsnmc>

COMPETITION

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This branch is 14 commits ahead of scidash:master		
		Pull Request
2009a test now runs against hand-coded LIF model		
 rgerkin	authored 7 days ago	latest commit e73962fd32
 capabilities	2009a test now runs against hand-coded LIF model	7 days ago
 comparators	2009a test now runs against hand-coded LIF model	7 days ago
 docs	Added documentation for spike train similarity metric	23 days ago
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 records	Initial commit	a year ago
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- We aim to solve these with *unit testing philosophy + domain standards*

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 - Observed data for test parameterization retrieved automatically from trusted data repositories.

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 - Being replaced by ElectroPhysiology Analysis Toolkit (*ElePhAnT*)

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 - Synaptic: ?

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Published literature

Novel subcellular distribution pattern of A-type K⁺ channels on neuronal surface.

Unique clustering of A-type potassium channels on different cell types of the main olfactory bulb.

Kollo M, Holderith N, Antal M, Nusser Z.
Theoretical and functional studies predicted a highly non-uniform distribution of voltage-gated ion channels on the neuronal surface. This was confirmed by recent immunolocalization experiments for Na⁺, Ca²⁺, hyperpolarization activated mixed cation and K⁺ channels. These experiments also indicated that some K⁺ channels were clustered in synaptic or non-synaptic membrane specializations. Here we analysed the subcellular distribution of Kv4.2 and Kv4.3 subunits in the rat main olfactory bulb at high resolution to address whether clustering characterizes their distribution, and whether they are concentrated in synaptic or non-synaptic junctions. The cell surface distribution of the Kv4.2 and Kv4.3 subunits is highly non-uniform. Strong Kv4.2 subunit-immunopositive clusters were detected in intercellular junctions made by mitral, external tufted and granule cells (GCs). We also found Kv4.3 subunit-immunopositive clusters in periglomerular (PGC), deep short-axon and GCs. In the juxtaglomerular region some calretinin-immunopositive glial cells enwrap neighboring PGC somata in a cap-like manner. Kv4.3 subunit clusters are present in the cap membrane that directly contacts the PGC, but not the one that faces the neuropil. In membrane specializations established by members of the same cell type, K⁺ channels are enriched in both membranes, whereas specializations between different cell types contain a high density of channels asymmetrically. None of the K⁺ channel-rich junctions showed any of the ultrastructural features of known chemical synapses. Our study provides evidence for highly non-uniform subcellular distributions of A-type K⁺ channels and predicts their involvements in novel

Physiology database

Olfactory Bulb Mitral Cell

Input resistance	200 MΩ
V _{rest}	-65 mV
Spike width	1 ms
...	

CA1 Pyramidal Cell

Input resistance	400 MΩ
V _{rest}	-70 mV
Spike width	.5 ms
...	

Extracted from Literature

NEUROELECTRO

```
In [1]: from neuronunit.neuroelectro import NeuroElectroSummary
```

```
In [2]: summary = NeuroElectroSummary(neuron={'name':'Hippocampus CA1 Pyramidal Cell'},  
...: ephysprop={'name':'spike width'})
```

```
In [3]: observation = summary.get_observation(show=True)
```

Getting data values from neuroelectro.org

http://www.neuroelectro.org/api/1/nes/?e__name=spike+width&n__name=Hippocampus+CA1+Pyramidal+Cell

```
{u'e': {u'definition': u'Duration of AP, not explicitly referred to as half-width',  
u'id': 23,  
u'name': u'spike width',  
u'nlex_id': None,  
u'norm_criteria': u'Values are unchanged from those reported. Values currently lump multiple measures of spike width which do not  
explicitly denote spike half-width. Refer to individual articles for definition and calculation methodology.'},  
u'n': {u'id': 85,  
u'name': u'Hippocampus CA1 pyramidal cell',  
u'neuron_db_id': 258,  
u'nlex_id': u'sao830368389'},  
u'num_articles': 6,  
u'num_nedms': 10,  
u'value_mean': 2.602083333333333,  
u'value_sd': 0.766070080381394}
```

```
In [4]: from neuronunit.tests import SpikeWidthTest
```

```
In [5]: ca1_pyramidal_spike_width_test = SpikeWidthTest(observation = observation)
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'n': {'id': 85,  
'name': 'Hippocampus CA1 pyramidal cell',  
'neuron_db_id': 258,  
'nlex_id': 'sao830368389'},  
'num_articles': 6,  
'num_nedms': 10,  
'value_mean': 2.602083333333333,  
'value_sd': 0.766070080381394}
```

```
In [4]: from neuronunit.tests import SpikeWidthTest
```

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In [5]: ca1_pyramidal_spike_width_test = SpikeWidthTest(observation = observation)
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- Uses the NeuroElectro API (and NeuroLex) to get collated data about a named *neuron type* for a specified *electrophysiological property* to parameterize a test.

NEUROELECTRO

```
In [1]: from neuronunit.neuroelectro import NeuroElectroSummary

In [2]: summary = NeuroElectroSummary(neuron={'name':'Hippocampus CA1 Pyramidal Cell'},
...:                               ephysprop={'name':'spike width'})

In [3]: observation = summary.get_observation(show=True)
Getting data values from neuroelectro.org
http://www.neuroelectro.org/api/1/nes/?e__name=spike+width&n__name=Hippocampus+CA1+Pyramidal+Cell
{u'e': {u'definition': u'Duration of AP, not explicitly referred to as half-width',
        u'id': 23,
        u'name': u'spike width',
        u'nlex_id': None,
        u'norm_criteria': u'Values are unchanged from those reported. Values currently lump multiple measures of spike width which do not explicitly denote spike half-width. Refer to individual articles for definition and calculation methodology.'},
 u'n': {u'id': 85,
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 - Simulation description: *SED-ML* (<http://sed-ml.org>)
 - Simulation execution: ... whatever reads NeuroML (neuroConstruct, NEURON, etc.)

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... followed by many interactions with this model via its capabilities, in the course of test execution.

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 - If your model platform has a helper class (e.g. *NeuroConstructModel*) you are ready to go!
 - If not, implement the required capabilities (i.e. mostly just wrapping the existing functionality of your model in capability methods).

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 - Look your child in the face when they ask if you, an alleged scientist, used the scientific method in the development of your model.

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 - It could become the gold standard by which models are judged!

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 - Does the worm sim swim like the real worm?

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