OSB Automated Model Validation

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**Status**

Note: this table is still in development!

These status values are currently based on a manual curation process, scoring the models on the completeness of the translation of the model from the original format to NeuroML (or PyNN).

For simulators, the score represents how well the model translates to the specific simulator from the simulator independent format, NOT the availability of original scripts in that simulator.

The longer term aim is to have these scores generated automatically from tests based on parsing of the NeuroML and comparison to expected model behaviour.

<table>
<thead>
<tr>
<th>Model Name</th>
<th>Curation</th>
<th>NeuroML v1.x</th>
<th>NeuroML v2.x</th>
<th>PyNN</th>
<th>NEURON</th>
<th>GENESIS 2</th>
<th>MOOSE</th>
<th>PSICS</th>
<th>NEST</th>
<th>Brian</th>
<th>OSB Model Validation</th>
</tr>
</thead>
<tbody>
<tr>
<td>OSB vogelsetal2011</td>
<td>★★★</td>
<td></td>
<td></td>
<td></td>
<td>★★★</td>
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<tr>
<td>OSB blender-to-neuroml</td>
<td>★</td>
<td></td>
<td></td>
<td></td>
<td>★★★</td>
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<tr>
<td>OSB bluhive-showcase</td>
<td>★★★</td>
<td>★★★</td>
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<td>★★★</td>
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<tr>
<td>OSB briansshowcase</td>
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<td>★★★</td>
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<tr>
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<td></td>
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<td>★★★</td>
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<tr>
<td>User nc_superdeep</td>
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<tr>
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<td>★</td>
<td>★★★</td>
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<tr>
<td>OSB dentate</td>
<td>★</td>
<td>★★</td>
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<td></td>
<td>★★★</td>
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<td>OSB drosophila-acc-I3-motoneuron-gunay-et-al-2014</td>
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<td>★★</td>
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<td>★★★</td>
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<tr>
<td>OSB fitzhugh-nagumo-fitzhugh-1969</td>
<td>★</td>
<td>★★★</td>
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<td>OSB fpgashowcase</td>
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</tbody>
</table>
Our motivations

- Manual curation / Subjective star rating
- Some form of “quality control” for OSB models
- Concrete example: how accurate are NeuroML translations?
- The danger of blindly using software
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Retraction of Reyes and Chang, Science 308 (5724) 1028-1031.
Retraction of Chang and Roth, Science 293 (5536) 1793-1800.

Science 22 December 2006:
Vol. 314 no. 5807 p. 1875
DOI: 10.1126/science.314.5807.1875b

LETTERS

Retraction

We wish to retract our research article "structure of MsbA from E. coli: A homolog of the multidrug resistance ATP binding cassette (ABC) transporters" and both of our Reports "Structure of the ABC transporter MsbA in complex with ADP-vanadate and lipopolysaccharide" and "X-ray structure of the EmrE multidrug transporter in complex with a substrate" (1-3).

The recently reported structure of Sav1866 (4) indicated that our MsbA structures (1, 2, 5) were incorrect in both the hand of the structure and the topology. Thus, our biological interpretations based on these inverted models for MsbA are invalid.

An in-house data reduction program introduced a change in sign for anomalous differences. This program, which was not part of a conventional data processing package, converted the anomalous pairs (I+ and I-) to (F- and F+), thereby introducing a sign change. As the diffraction data collected for each set of MsbA crystals and for the EmrE crystals were processed with the same program, the structures reported in (1-3, 5, 6) had the wrong hand.

The error in the topology of the original MsbA structure was a consequence of the low resolution of the data as well as breaks in the electron density for the connecting loop regions. Unfortunately, the use of the multicycopy refinement procedure still allowed us to obtain reasonable refinement values for the wrong structures.
OSB projects are dynamic

- Does a new model version behave as “expected”?
- Back our claims: does the code *really* produce figure 7?
- Will the model behave the same in different environments?
  - *tabula rasa* environment for testing
  - (another approach: Andrew Davison’s *sumatra*)
Validation/Testing: “Quality control”

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- **Zeroth order validation:**
  - Is the model doing what we claim it to do?
  - Sanity checking
    - activation variables, concentrations, temperatures...
  - Are different implementations producing the same results?
  - Comparing distinct models is a “higher order” goal
    - Richard Gerkin’s *neurounit* / *sciunit*
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Guidelines

- Simple to use and setup. Declarative format, no logic
- Automated testing for new commits (*continuous integration*)
- Extensible (adding new tests/backends)
How does it look like a
proof-of-concept implementation!
expect changes!

- https://github.com/borismarin/hh-testing
- https://travis-ci.org/borismarin/hh-testing
How to enable it for a project

1. Dry-run test file (*omt* extension)

   ```
   engine: NEURON
   target: NEURON/script.hoc
   ```

2. Add our `.travis.yml` file to the repo

OR

1. Install our python package
2. Follow the wizard: `omv_autogen`
Model Emergent Properties [*mep*] files

<table>
<thead>
<tr>
<th>system: Classical HH model</th>
</tr>
</thead>
<tbody>
<tr>
<td>experiments:</td>
</tr>
<tr>
<td>experiment 1, autonomous activity:</td>
</tr>
<tr>
<td>expected:</td>
</tr>
<tr>
<td>resting: -64.9</td>
</tr>
<tr>
<td>morphology:</td>
</tr>
<tr>
<td>total area: 157080</td>
</tr>
<tr>
<td>number of cells: 1</td>
</tr>
<tr>
<td>temperature: 6.3</td>
</tr>
</tbody>
</table>

- We need to specify our expectations
- Information that comes from the model after computations
- Can be used to generate visual summary
## OSB Model Test

**target:** hhnostim.hoc  
**engine:** NEURON  
**implements:**  
  - mep: ../hh.mep  
**experiment:** experiment 1, autonomous activity  
**observables:**  
  - **resting:**  
    - **file:**  
      - **path:** /tmp/nrnhhnostim.dat  
      - **columns:** [0,1]  
      - **average last:** 100  
      - **tolerance:** 1e-2  
  - **morphology:**  
    - **base section:** soma

- Given a *mep* file, specify mappings to implementation  
- how to “run”  
- how/where info is stored
Under development

- More tests!
  - BTW, what should we test for?
- More backends!
- Coupling to NeuroML exporters:
  - “download as…” available if test passes
- Unit handling
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