NeuroML update

Ankur Sinha

21/09/2022

What we've been up to on the NeuroML front

- Google summer of code (GSoC)
- Paper and general improvements

Google Summer of Code

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  - Conversions of models to NeuroML (to allow them to be re-used and featured on OSB)
  - Get folks looking into and using NeuroML in different use cases
  - Get folks to improve NeuroML where possible

GSoC: Anuja: convert Allen Institute models to NeuroML

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- Steps:
  - Automate download of models using the Allen SDK
  - Automate conversion to NeuroML
  - Plot comparison graphs to validate conversions (LIF models, Detailed)
  - Document comparison, usage, update OMV tests for CI

GSoC: Anuja: example figure I

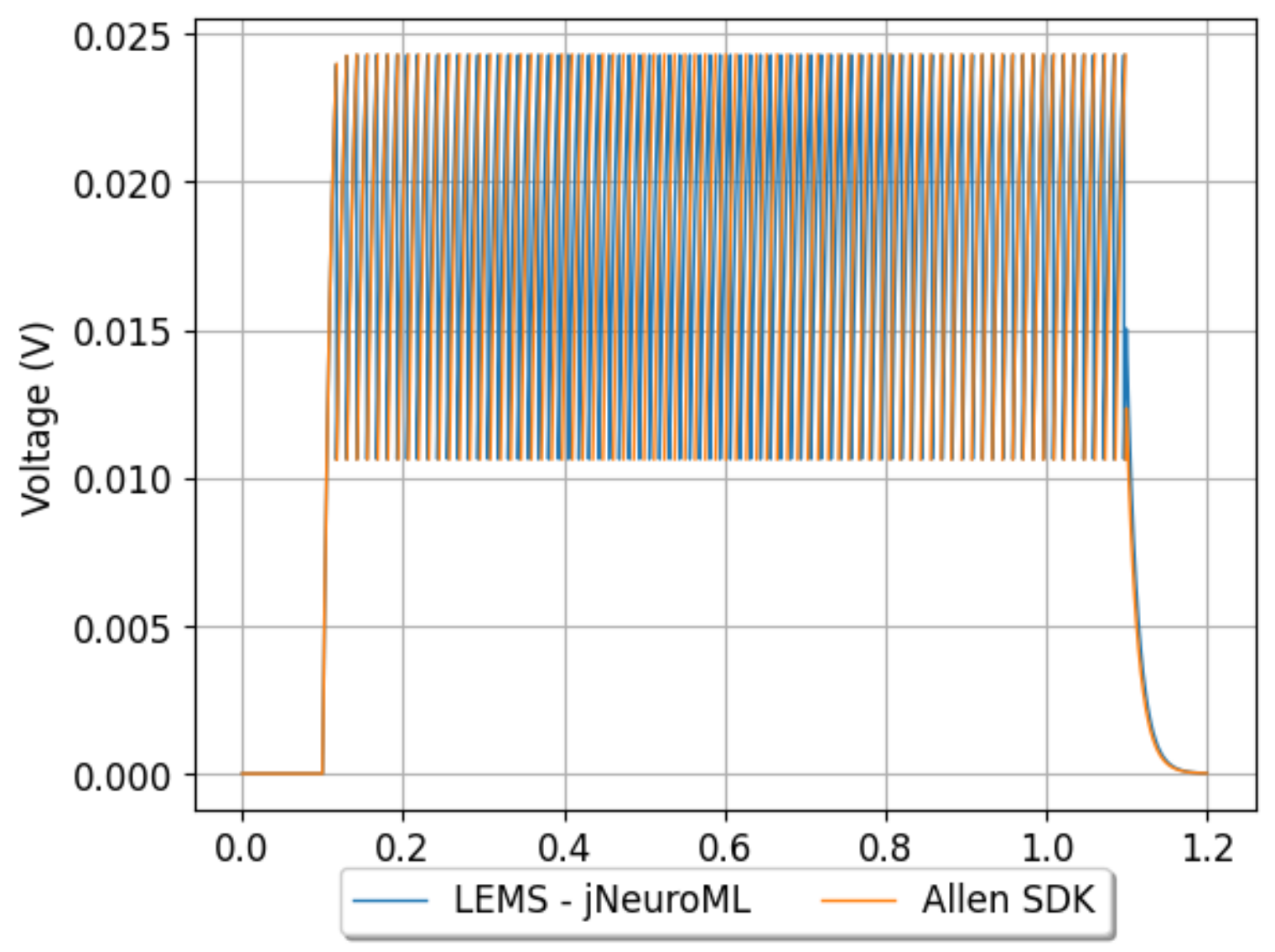

Figure 1: Membrane potentials of Allen and NeuroML models

GSoC: Anuja: example figure II

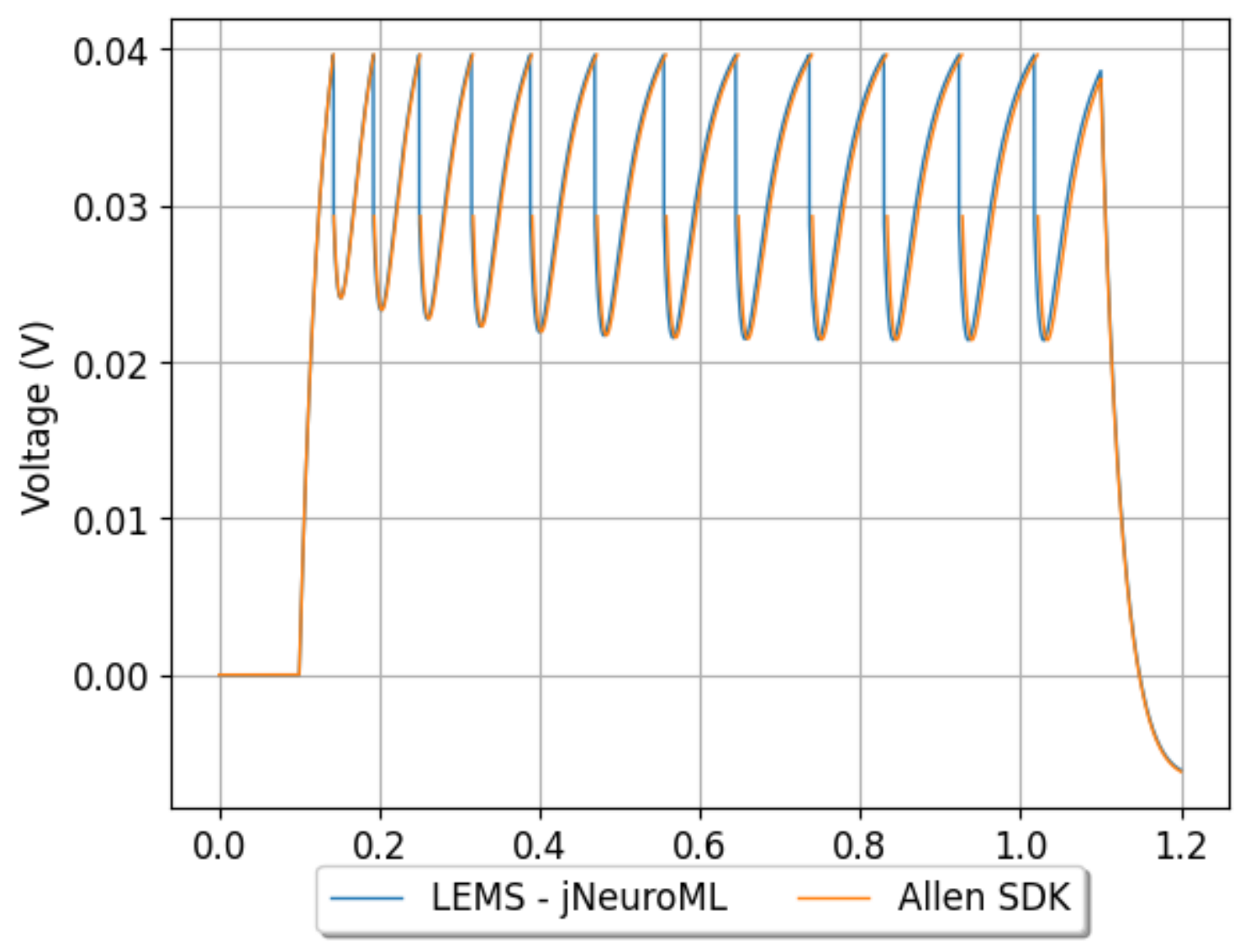

Figure 2: Membrane potentials of Allen and NeuroML models

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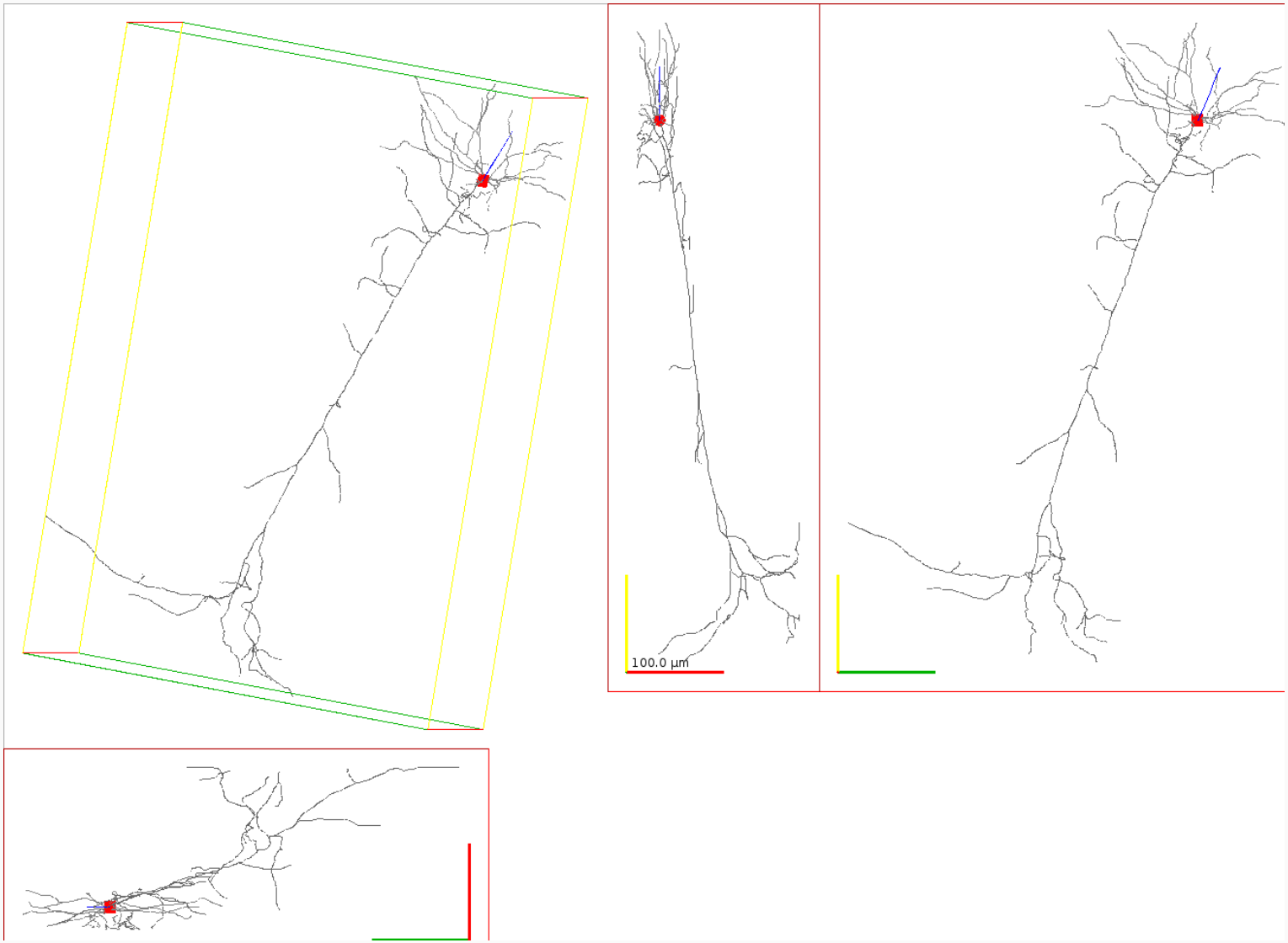

Figure 3: Morphology of example cell

GSoC: Anuja: example figure IV

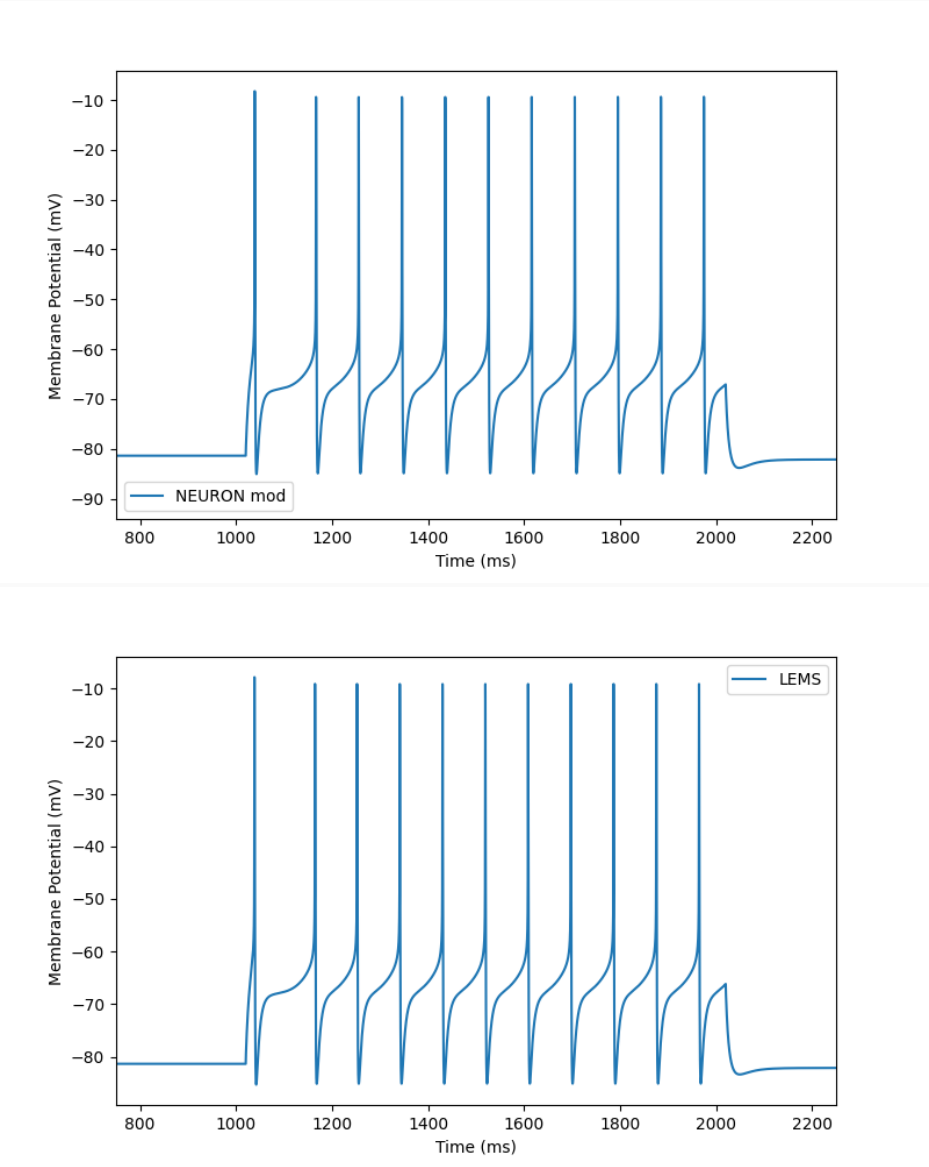

Figure 4: NEURON vs NeuroML output

GSoC: Shayan: convert BahlEtAl2012 (Reduced L5 Pyr Cell) to NeuroML

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- Source models: OSB/BahlEtAl2012

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- MSc/BSc from IIT Kharagpur (Maths and Computing)
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- Steps:
  - Convert ion channels to NeuroML, validate, compare with NEURON mod files
  - Implement single compartment cell model with passive channels
    - incrementally add ion channels
    - compare with NEURON model
  - Implement multi-compartmental cell, repeat
  - Document comparison, usage, update OMV tests for CI
  - Interactive notebook to reproduce figures from paper using NeuroML models

GSoC: Shayan: example figures

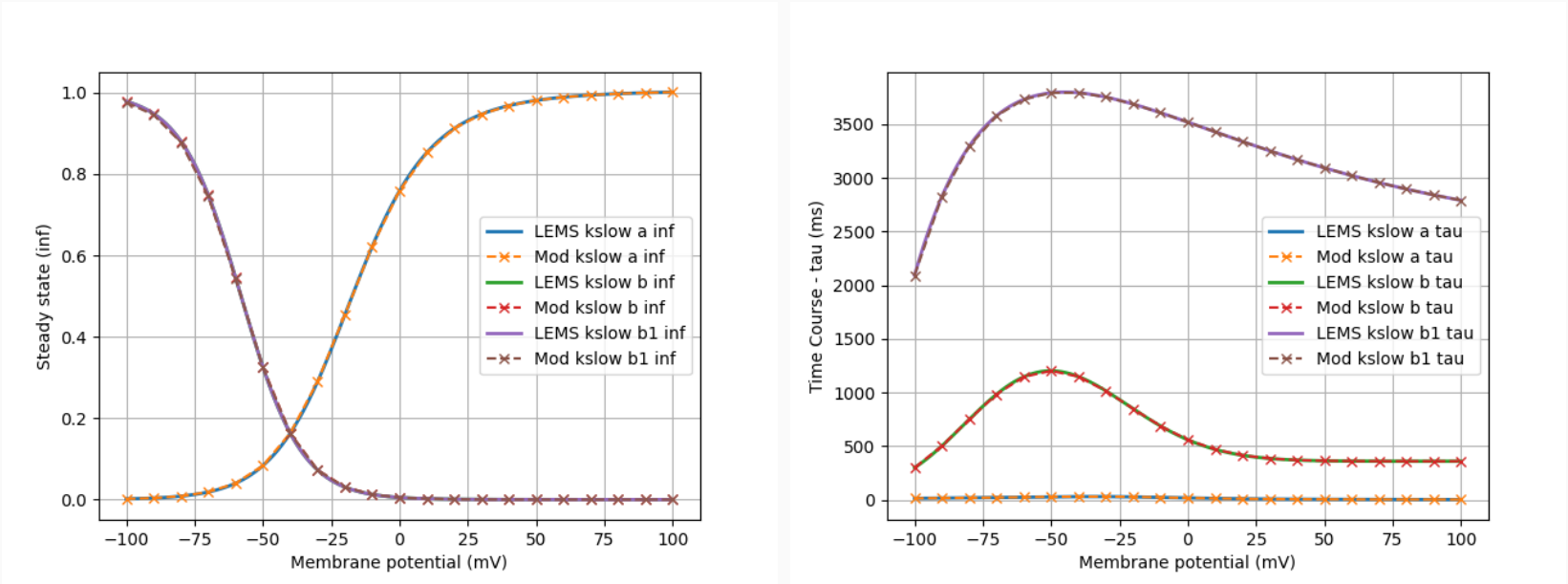

Figure 5: Comparing ion channels: steady state, time constant

GSoC: Shayan: example figures II

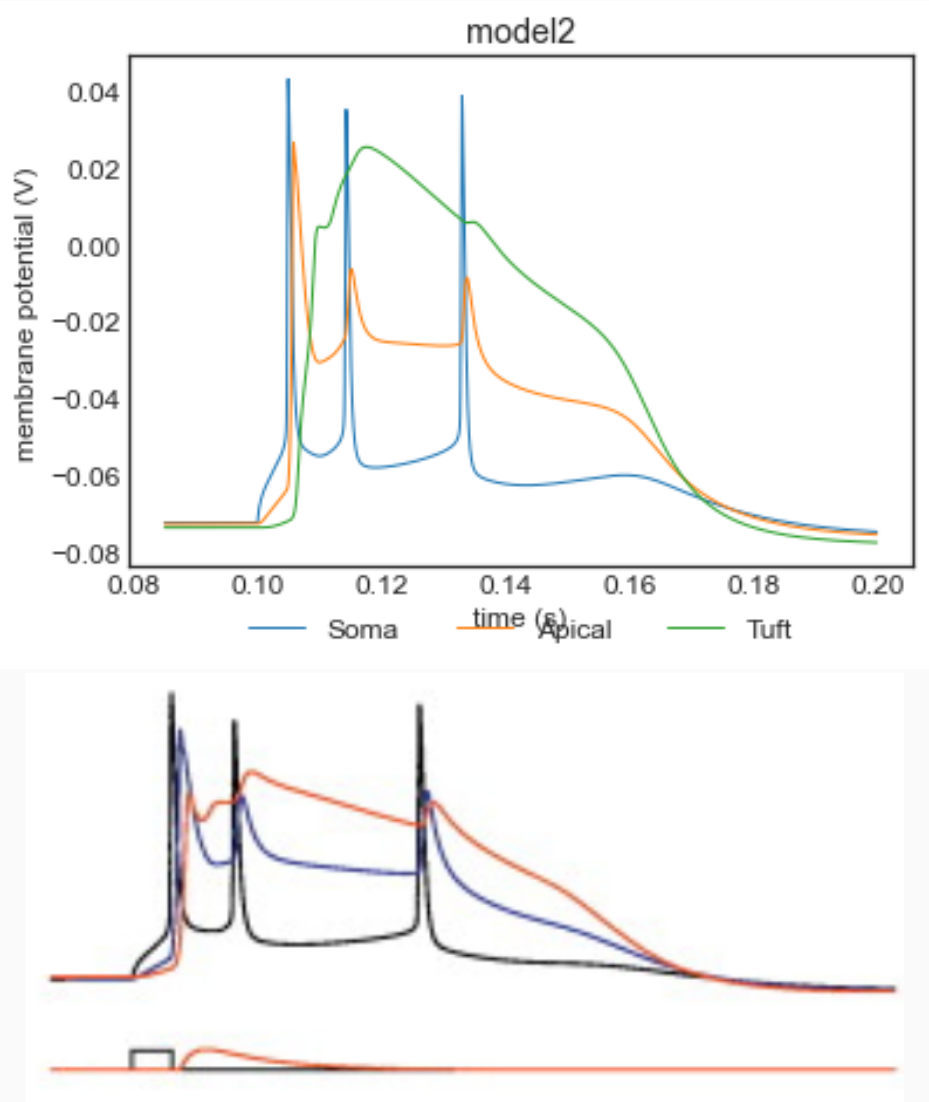

Figure 6: Replicating figures from the paper (8d)

GSoC: Rahul: convert HH tutorial to Jupyter notebook

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- Aerospace engineer (MTech, IIT Kharagpur), working in South Korea
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- Steps:
  - Investigate Jupyter widgets
  - Convert pure Python HH tutorial to use Jupyter widgets
  - Investigate NeuroML based tutorial
  - Investigate conversion of NeuroML to Jupyter widgets
  - Update sphinx documentation for ReadTheDocs site
  - Document usage.

GSoC: Rahul: example I

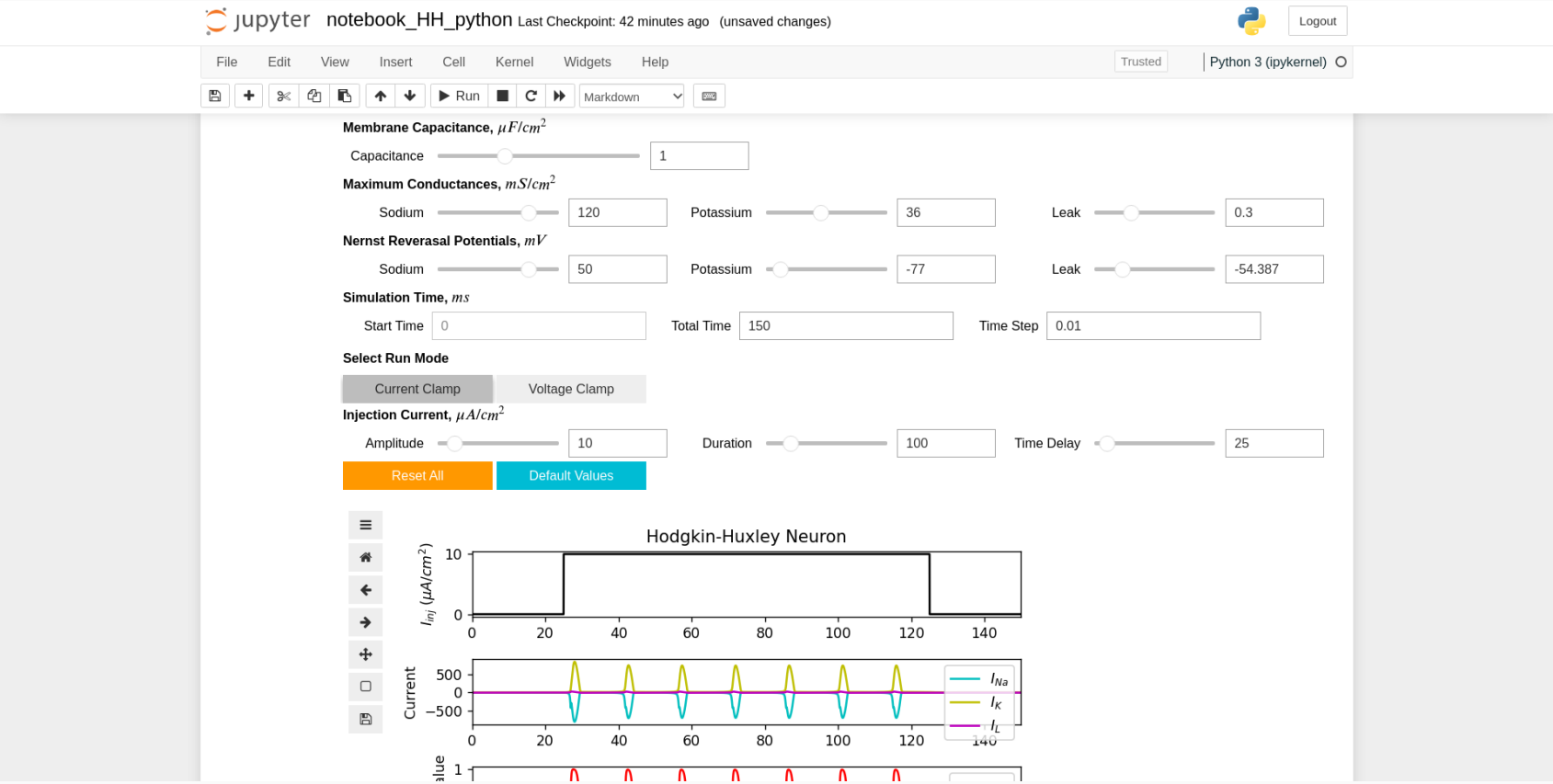

Figure 7: Pure python tutorial converted to use Jupyter Widgets

GSoC: Rahul: example II

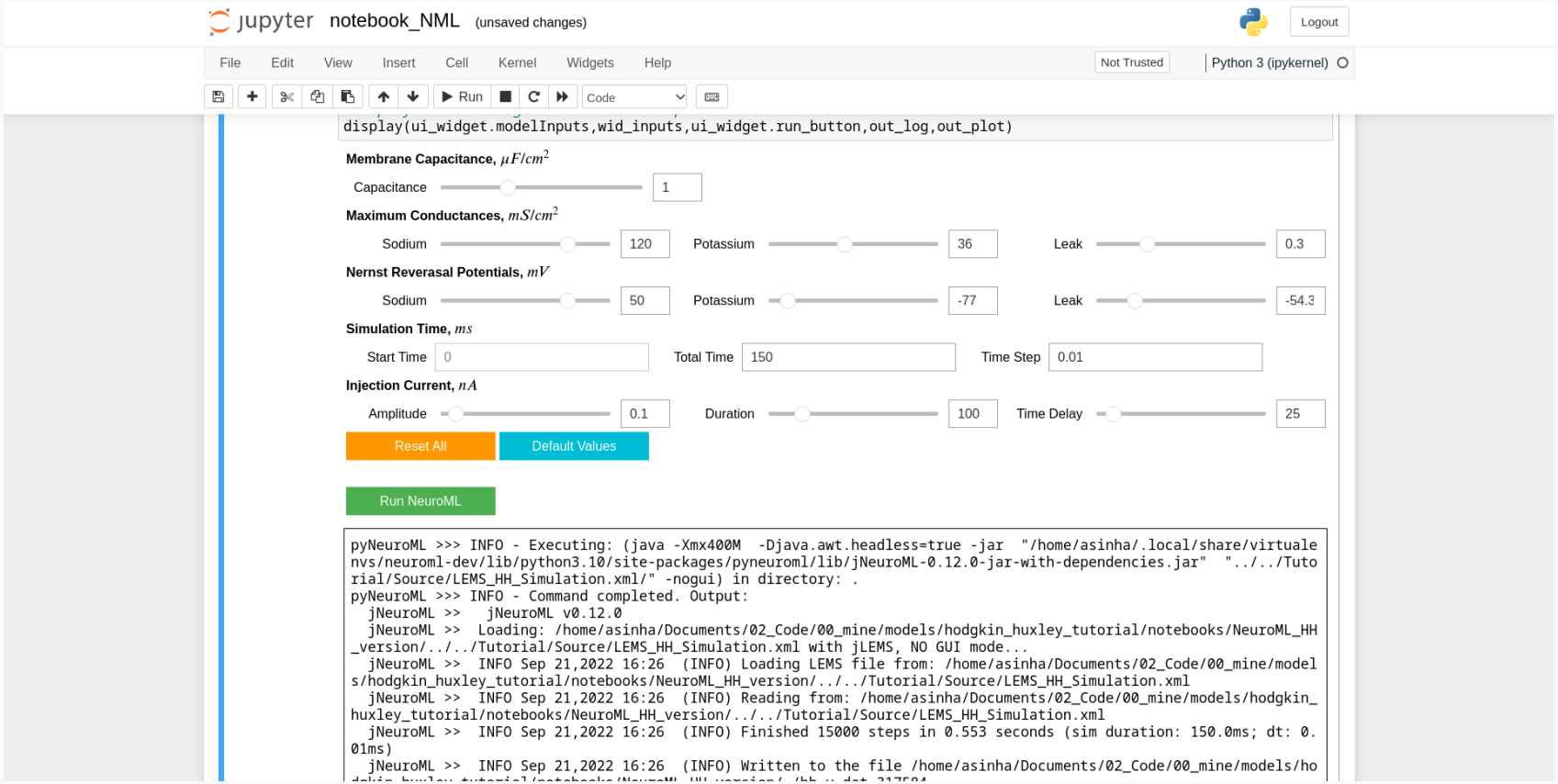

Figure 8: NeuroML tutorial converted to use Jupyter Widgets

Paper and general updates

Paper: NeuroML is the best thing since sliced bread

Convince readers (research community) to use NeuroML for their modelling work*.

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Convince readers (research community) to use NeuroML for their modelling work*.

- *instead/ahead of other tools
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  - not as an afterthought for standardisation—once the paper has been published no one has time to re-write model (or re-process data!) to standardise
    - the carrot, “standardisation is good for science”, isn’t enough in a mostly resource limited academic/research system
    - requires stick: “for this grant, you must . . . ”; “for this journal, you must . . . ”

You should use NeuroML because

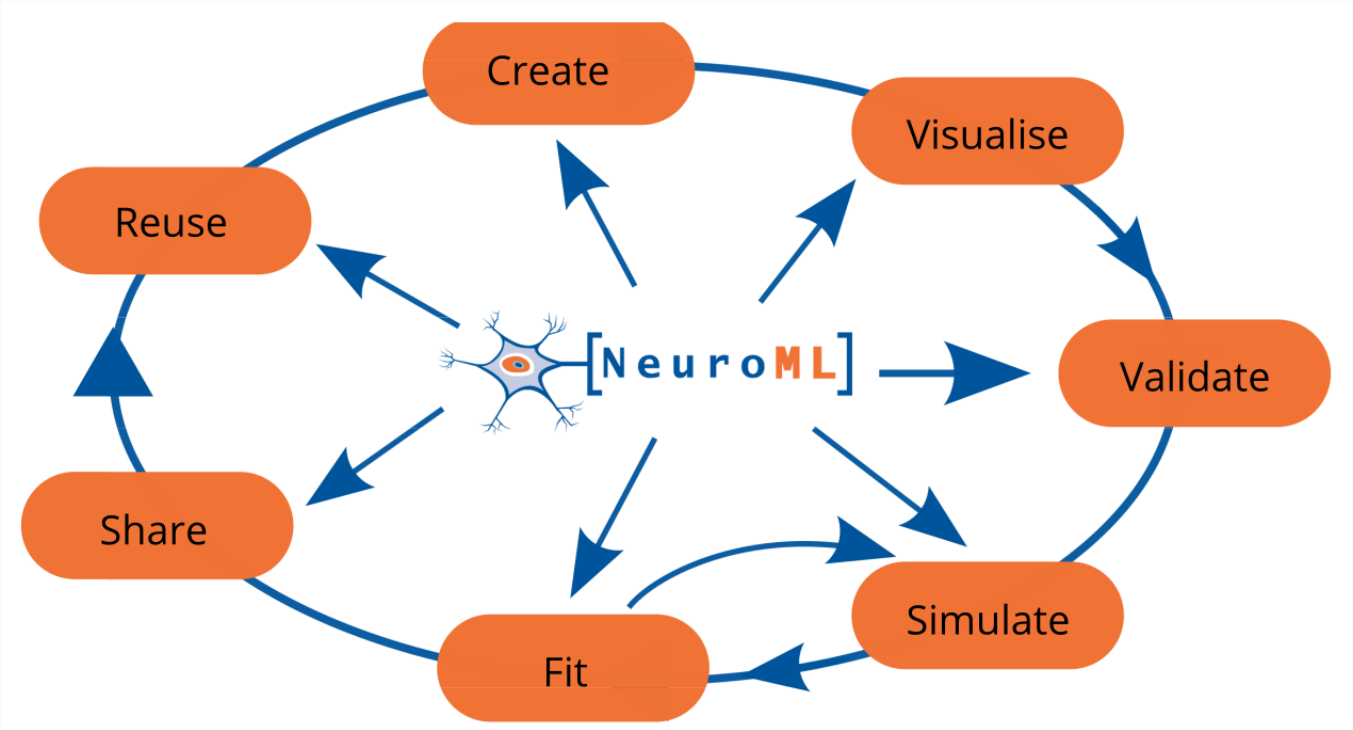

Figure 9: NeuroML overview figure from paper

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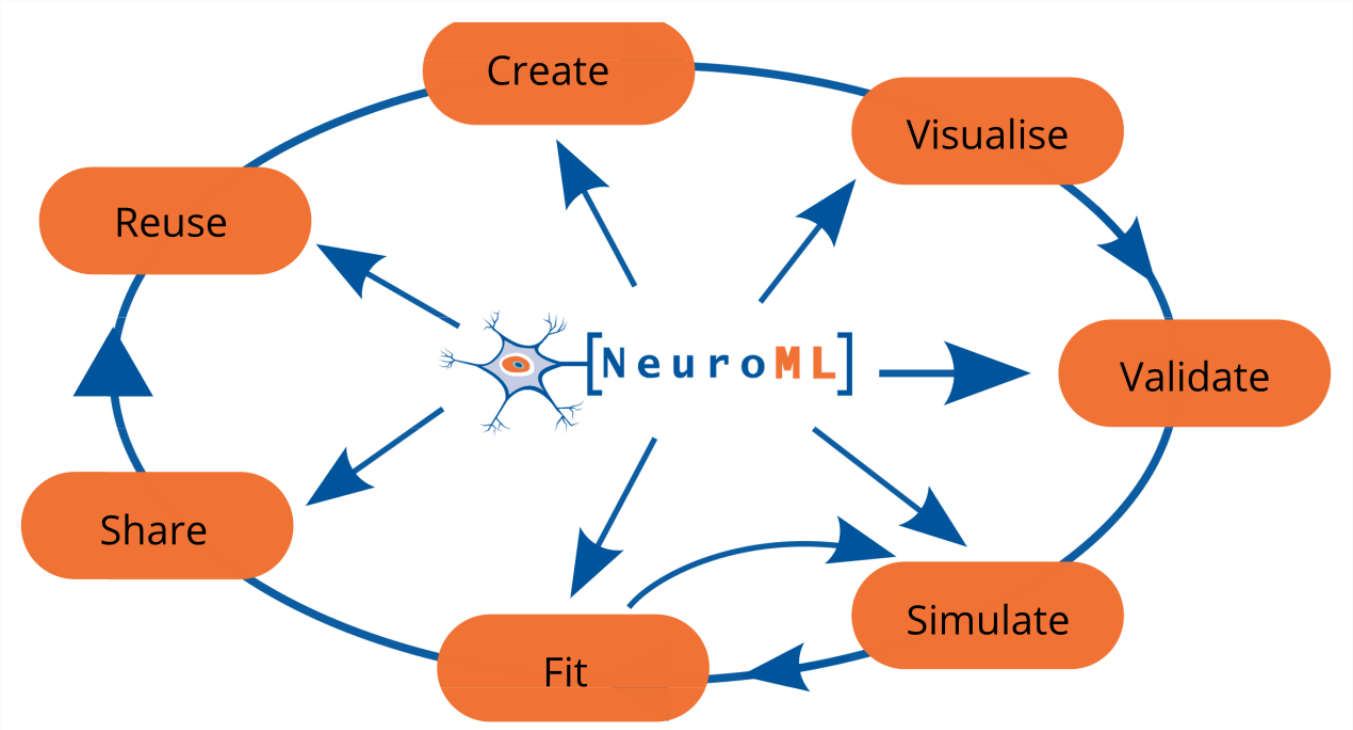

Figure 9: NeuroML overview figure from paper

These claims are all true, and have been for quite a while.

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- information on NeuroML needs to be easy to find:
  - website
    - point of entry for completely new users: first impression
    - replaced with modern looking static page that redirects to individual pages in docs
    - all information migrated to docs

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    - point of entry for completely new users: first impression
    - replaced with modern looking static page that redirects to individual pages in docs
    - all information migrated to docs
  - docs
    - re-organised, modernised
    - include tutorials, interactive tutorials via Jupyter note books, how-tos
    - complete searchable schema docs
    - still not yet fully complete

So many advantages: why isn't everyone using it?

Irrespective of all its features, NeuroML needs to be easier to use than other tools.

- usability: so much can be done, but can it be done easily?
  - has not been clearly easier to use than other tools
  - Python API exists, but we haven't taken advantage of it enough to make life easier for users yet

Example: create: single neuron Izhikevich network (from docs)

```
nml_doc = NeuroMLDocument(id="IzhSingleNeuron")

izh0 = Izhikevich2007Cell(
    id="izh2007RS0", v0="-60mV", C="100pF", k="0.7nS_per_mV", vr="-60mV",
    vt="-40mV", vpeak="35mV", a="0.03per_ms", b="-2nS", c="-50.0mV", d="100pA")
nml_doc.izhikevich2007_cells.append(izh0)

net = Network(id="IzhNet")
nml_doc.networks.append(net)

size0 = 1
pop0 = Population(id="IzhPop0", component=izh0.id, size=size0)
net.populations.append(pop0)

pg = PulseGenerator(
    id="pulseGen_%i" % 0, delay="0ms", duration="1000ms",
    amplitude="0.07 nA"
)
nml_doc.pulse_generators.append(pg)
exp_input = ExplicitInput(target="%s[%i]" % (pop0.id, 0), input=pg.id)
net.explicit_inputs.append(exp_input)

nml_file = 'izhikevich2007_single_cell_network.nml'
writers.NeuroMLWriter.write(nml_doc, nml_file)
print("Written network file to: " + nml_file)

validate_neuroml2(nml_file)
```

Inspect/visualise network

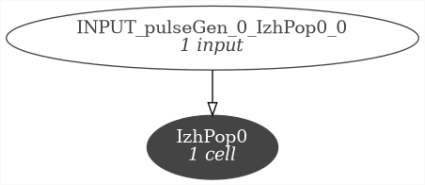


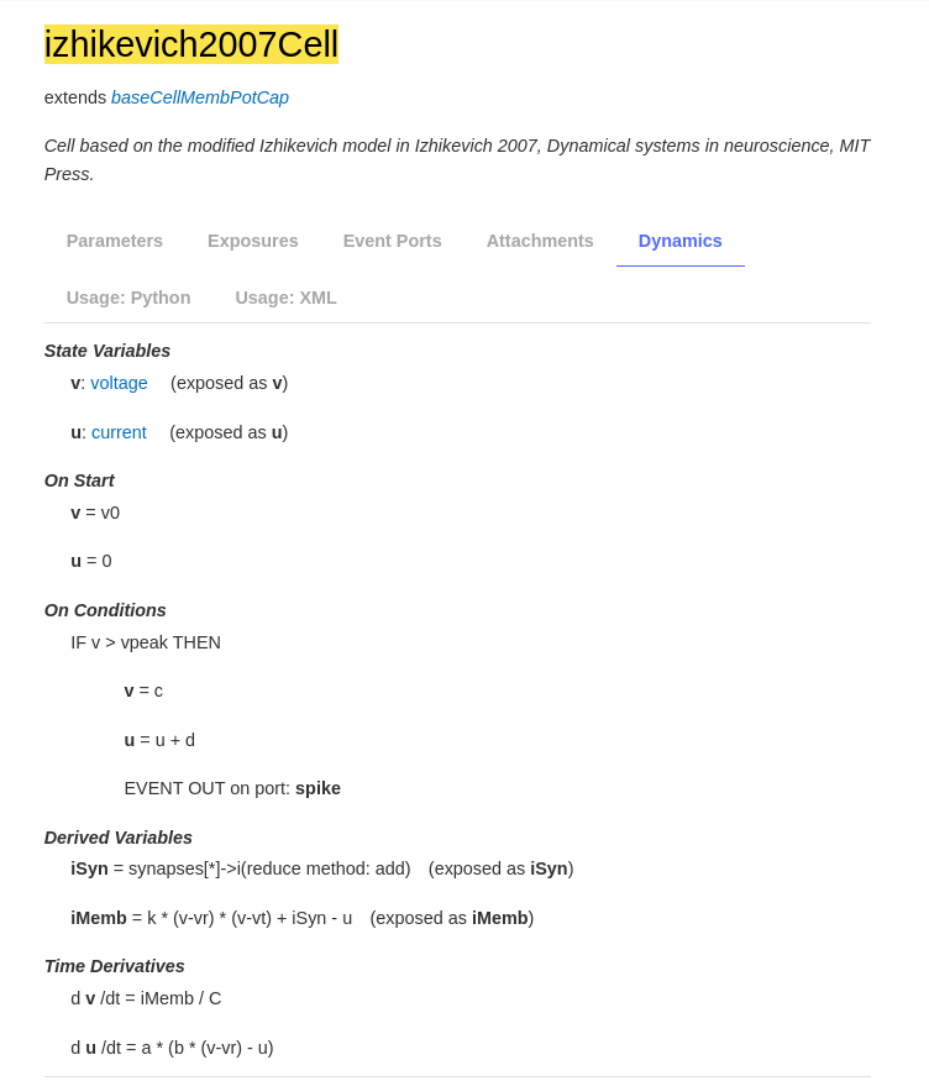
Figure 10: Generated network graph

```
>>> nml_doc.summary()
*********************************************************
* NeuroMLDocument: IzhSingleNeuron
*
*  Izhikevich2007Cell: ['izh2007RS0']
*  PulseGenerator: ['pulseGen_0']
*
*  Network: IzNet
*
*   1 cells in 1 populations
*     Population: IzhPop0 with 1 components of type izh2007RS0
*
*   0 connections in 0 projections
*
*   0 inputs in 0 input lists
*
*   1 explicit inputs (outside of input lists)
*     Explicit Input of type pulseGen_0 to IzhPop0(cell 0), destination: unspecified
*
*********************************************************
```

Strengths

- extremely declarative
  - components (Izhikevich2007Cell, Network, Population, PulseGenerator, ExplicitInput) clearly visible
  - components and dynamics fully, formally documented in schema docs
  - component parameters clearly visible
  - units/dimensions explicitly mentioned

Strengths



izhikevich2007Cell

extends *baseCellMembPotCap*

Cell based on the modified Izhikevich model in Izhikevich 2007, Dynamical systems in neuroscience, MIT Press.

Parameters | Exposures | Event Ports | Attachments | **Dynamics**

Usage: Python | Usage: XML

State Variables

v: voltage (exposed as **v**)

u: current (exposed as **u**)

On Start

v = v0

u = 0

On Conditions

IF v > vpeak THEN

v = c

u = u + d

EVENT OUT on port: **spike**

Derived Variables

iSyn = synapses[*]->i(reduce method: add) (exposed as **iSyn**)

iMemb = k * (v-vr) * (v-vt) + iSyn - u (exposed as **iMemb**)

Time Derivatives

d **v** /dt = iMemb / C

d **u** /dt = a * (b * (v-vr) - u)

Figure 11: Schema docs on Izhikevich2007Cell

Strengths

- validation without simulation (no simulator has this)
  - Level 1 validation: units/dimensions, structure of model checked against schema
  - Level 2 validation: extra “logical” checks

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- validation without simulation (no simulator has this)
  - Level 1 validation: units/dimensions, structure of model checked against schema
  - Level 2 validation: extra “logical” checks
- easy simulation with different simulators
- easy visualisation and inspection of model: network structure, connectivity matrices, LEMS simulation graph, morphology figures, model summary

Weaknesses

- information on components: must switch back and forth between docs and code
    - Not too bad: required for most simulators/programming languages

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  - Not too bad: required for most simulators/programming languages
- unclear how components fit together
  - how do I know that Network $\rightarrow$ Populations $\rightarrow$?
- Too many "under the hood" bits that users are expected to know:
  - `nml_doc.izhikevich2007_cells.append(izh0)`
  - how do users know this?
    - read the schema docs?
    - read the NeuroML Python API documentation?
    - read the NeuroML Python API source? (currently 64,000 lines of code)

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  - using `jnml`, so requires Java
  - better than errors on run, but still quite late

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- validation upon model completion
  - using `jnml`, so requires Java
  - better than errors on run, but still quite late
- NeuroML generated NEURON code is less performant than native NEURON code
  - because hand-written mod files can be optimised, while we rely on a template to generate them
  - TODO: optimisation of template

Example: create: single neuron Izhikevich network (devel)

```
nml_doc = component_factory("NeuroMLDocument", id="IzhSingleNeuron")
nml_doc.info(show_contents=True)

izh0 = nml_doc.add(
    "Izhikevich2007Cell",
    id="izh2007RS0", v0="-60mV", C="100pF", k="0.7nS_per_mV", vr="-60mV",
    vt="-40mV", vpeak="35mV", a="0.03per_ms", b="-2nS", c="-50.0mV", d="100pA")
izh0.info(show_contents=True)

net = nml_doc.add("Network", id="IzNet", validate=False)

size0 = 1
pop0 = net.add("Population", id="IzhPop0", component=izh0.id, size=size0)

pg = nml_doc.add(
    "PulseGenerator",
    id="pulseGen_%i" % 0, delay="0ms", duration="1000ms",
    amplitude="0.07 nA"
)
exp_input = net.add("ExplicitInput", target="%s[%i]" % (pop0.id, 0), input=pg.id)

nml_doc.validate(recursive=True)

nml_file = 'izhikevich2007_single_cell_network.nml'
writers.NeuroMLWriter.write(nml_doc, nml_file)
print("Written network file to: " + nml_file)
```

The component factory

- single factory function to create new components
- runs extra checks
  - are all arguments (parameters) correct?
  - is the component valid (level 1 validation for each component at build-time)?

```
>>> izh0 = component_factory("Izhikevich2007Cell")
ValueError: Validation failed:
- Izhikevich2007Cell (None): Required value v0 is missing
- Izhikevich2007Cell (None): Required value k is missing
- Izhikevich2007Cell (None): Required value vr is missing
- Izhikevich2007Cell (None): Required value vt is missing
- Izhikevich2007Cell (None): Required value vpeak is missing
- Izhikevich2007Cell (None): Required value a is missing
- Izhikevich2007Cell (None): Required value b is missing
- Izhikevich2007Cell (None): Required value c is missing
- Izhikevich2007Cell (None): Required value d is missing
- Izhikevich2007Cell (None): Required value C is missing
- Izhikevich2007Cell (None): Required value id is missing
```

The component factory

```
>>> izh0 = component_factory(
      "Izhikevich2007Cell",
      id="izh2007RS0", v0="-60mV", C="100pF", k="0.7nS_per_mV", vr="-60mV",
      vt="-40ms", vpeak="35mV", a="0.03per_ms", b="-2nS", c="-50.0mV", d="100pA")

ValueError: Validation failed:
 - Izhikevich2007Cell (izh2007RS0): Value "-40mS" does not match xsd pattern restrictions:
 ↪  [['^(-?([0-9]*(\\.[0-9]+)?)([eE]-?[0-9]+)?[\\s]*(V|mV))$']]]
```

New add method

- uses component factory to create a new component and run checks
- smart enough to know where the new element needs to go in the parent

```
izh0 = Izhikevich2007Cell(
    id="izh2007RS0", v0="-60mV", C="100pF", k="0.7nS_per_mV", vr="-60mV",
    vt="-40mV", vpeak="35mV", a="0.03per_ms", b="-2nS", c="-50.0mV", d="100pA")
nml_doc.izhikevich2007_cells.append(izh0)
```

vs

```
izh0 = nml_doc.add(
    "Izhikevich2007Cell",
    id="izh2007RS0", v0="-60mV", C="100pF", k="0.7nS_per_mV", vr="-60mV",
    vt="-40mV", vpeak="35mV", a="0.03per_ms", b="-2nS", c="-50.0mV", d="100pA")
```

Inspect each component individually

```
izh0.info(show_contents=True)
Izhikevich2007Cell -- Cell based on the modified Izhikevich model in Izhikevich 2007, Dynamical
↪  systems in neuroscience, MIT Press
Please see the NeuroML standard schema documentation at
↪  https://docs.neuroml.org/Userdocs/NeuroMLv2.html for more information.

Valid members for Izhikevich2007Cell are:
* b (class: Nml2Quantity_conductance, Required)
        * Contents ('ids'/<objects>): -2nS

* C (class: Nml2Quantity_capacitance, Required)
        * Contents ('ids'/<objects>): 100pF

* c (class: Nml2Quantity_voltage, Required)
        * Contents ('ids'/<objects>): -50.0mV

* d (class: Nml2Quantity_current, Required)
        * Contents ('ids'/<objects>): 100pA

* neuro_lex_id (class: NeuroLexId, Optional)
* metaid (class: MetaId, Optional)
* v0 (class: Nml2Quantity_voltage, Required)
        * Contents ('ids'/<objects>): -60mV

* id (class: NmlId, Required)
        * Contents ('ids'/<objects>): izh2007RS0
  ...
```

Component Type info without creating a new component: ctinfo

```
>>> ctinfo("ExpOneSynapse")
ExpOneSynapse -- Ohmic synapse model whose conductance rises instantaneously by ( **gbase**  *
↪  **weight**  ) on receiving an event, and which decays exponentially to zero with time course
↪  **tauDecay**

Please see the NeuroML standard schema documentation at
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Valid members for ExpOneSynapse are:
* neuro_lex_id (class: NeuroLexId, Optional)
* gbase (class: Nml2Quantity_conductance, Required)
* metaid (class: MetaId, Optional)
* erev (class: Nml2Quantity_voltage, Required)
* notes (class: xs:string, Optional)
* id (class: NmlId, Required)
* properties (class: Property, Optional)
* annotation (class: Annotation, Optional)
* tau_decay (class: Nml2Quantity_time, Required)
```

Where does this component type fit?

```
>>> ctparentinfo("HHRate")
Please see the NeuroML standard schema documentation at
↪  https://docs.neuroml.org/Userdocs/NeuroMLv2.html for more information.

Valid parents for HHRate are:
* GateHHRates
        * forward_rate (class: HHRate, Required)
        * reverse_rate (class: HHRate, Required)
* GateHHRatesInf
        * forward_rate (class: HHRate, Required)
        * reverse_rate (class: HHRate, Required)
* GateHHRatesTau
        * forward_rate (class: HHRate, Required)
        * reverse_rate (class: HHRate, Required)
* GateHHRatesTauInf
        * forward_rate (class: HHRate, Required)
        * reverse_rate (class: HHRate, Required)
* GateHHUndetermined
        * forward_rate (class: HHRate, Optional)
        * reverse_rate (class: HHRate, Optional)
```

Additions to make multi-compartment cell building easier

- `set_init_memb_potential()` instead of

  `cell.biophysical_properties.membrane_properties.init_memb_potential`

- `add_channel_density()...`
- `add_segment`, `add_unbranched_segment_list...`
  - also takes care of NeuroLex (now InterLex) Ids, used by NEURON to create “sections”.
  - another hidden feature of NeuroML

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    - NeuroMLLite GUI (NeuroML v3?)
        - Will absorb all neuroConstruct functionality

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- Complete NetPyNE UI interactions with NeuroML
  - import works, but cannot modify model
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- Migrate all code to Python (so no more Java required)
  - long term, multi-year project, requires another grant