Multi-compartmental and multi-scale modeling in MOOSE via Python

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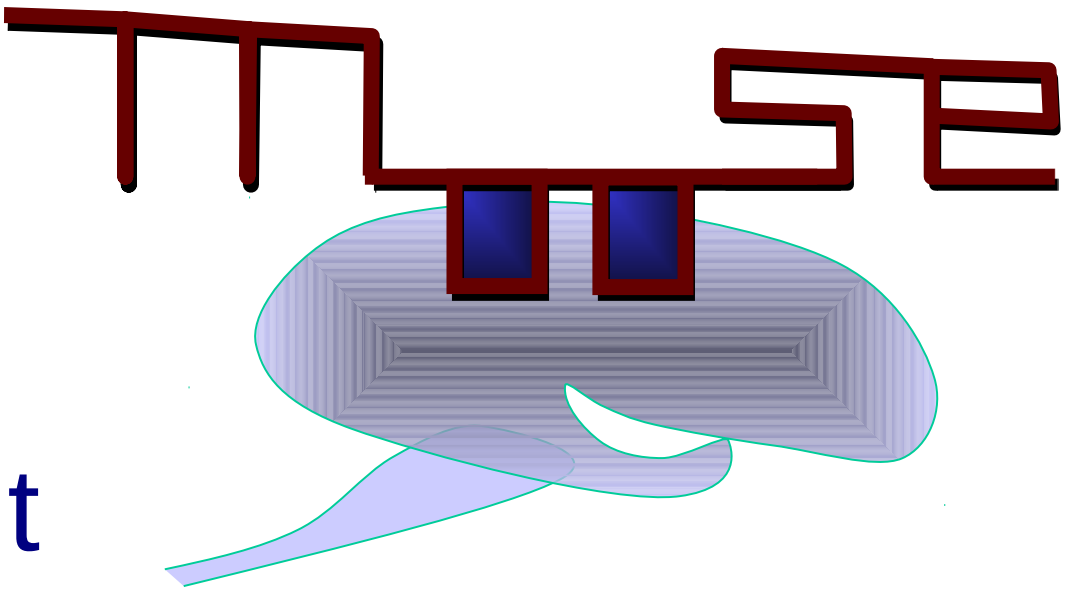
Outline

- Walk through: simple compartmental model
- Multiscale modeling outline
- Architecture of MOOSE
- Extensions
- Preview of upcoming version
- Future directions

the **M**ultiscale **O**bject-**O**riented **S**imulation **E**nvironment



Logo credit: Upi Bhalla

- A general purpose simulator framework
- Draws from experience with GENESIS

What is MOOSE?

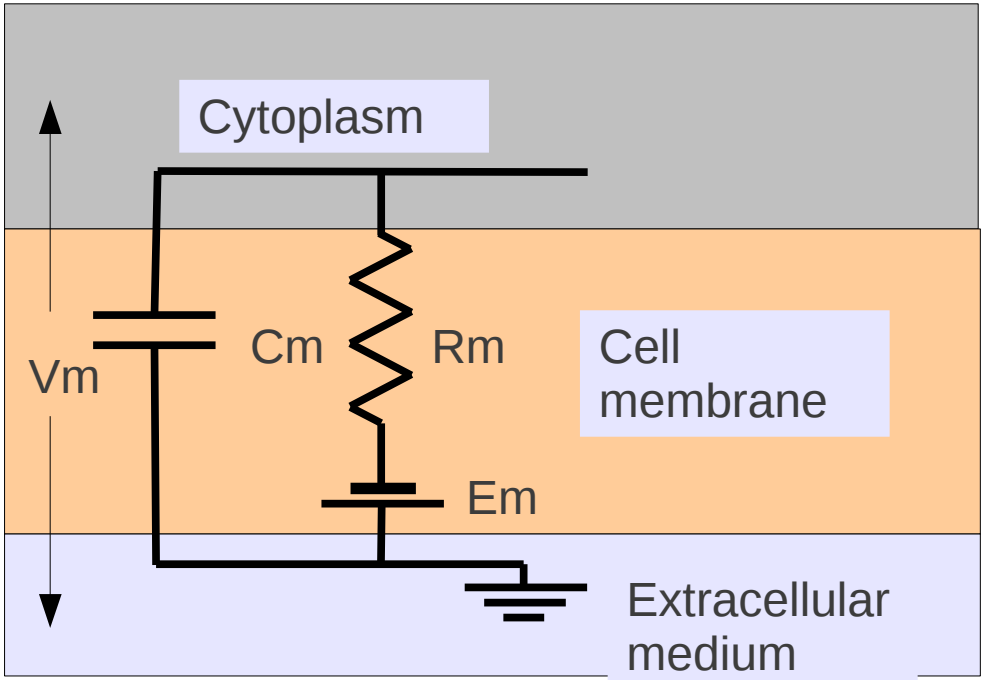
Depends on what *you* are and where you look.

A single passive compartment

```
import moose
soma = moose.Compartment('soma')
soma.Rm = 7.6e6
soma.Cm = 7e-9
soma.Em = -70e-3
soma.inject = 1e-6
```

- Getting help:

```
moose.doc('Compartment')
moose.doc('HHChannel.channel')
```



Recording data

```
vm_table = moose.Table('/vm')

vm_table.stepMode = 3

vm_table.connect('inputRequest',
soma, 'Vm')
```

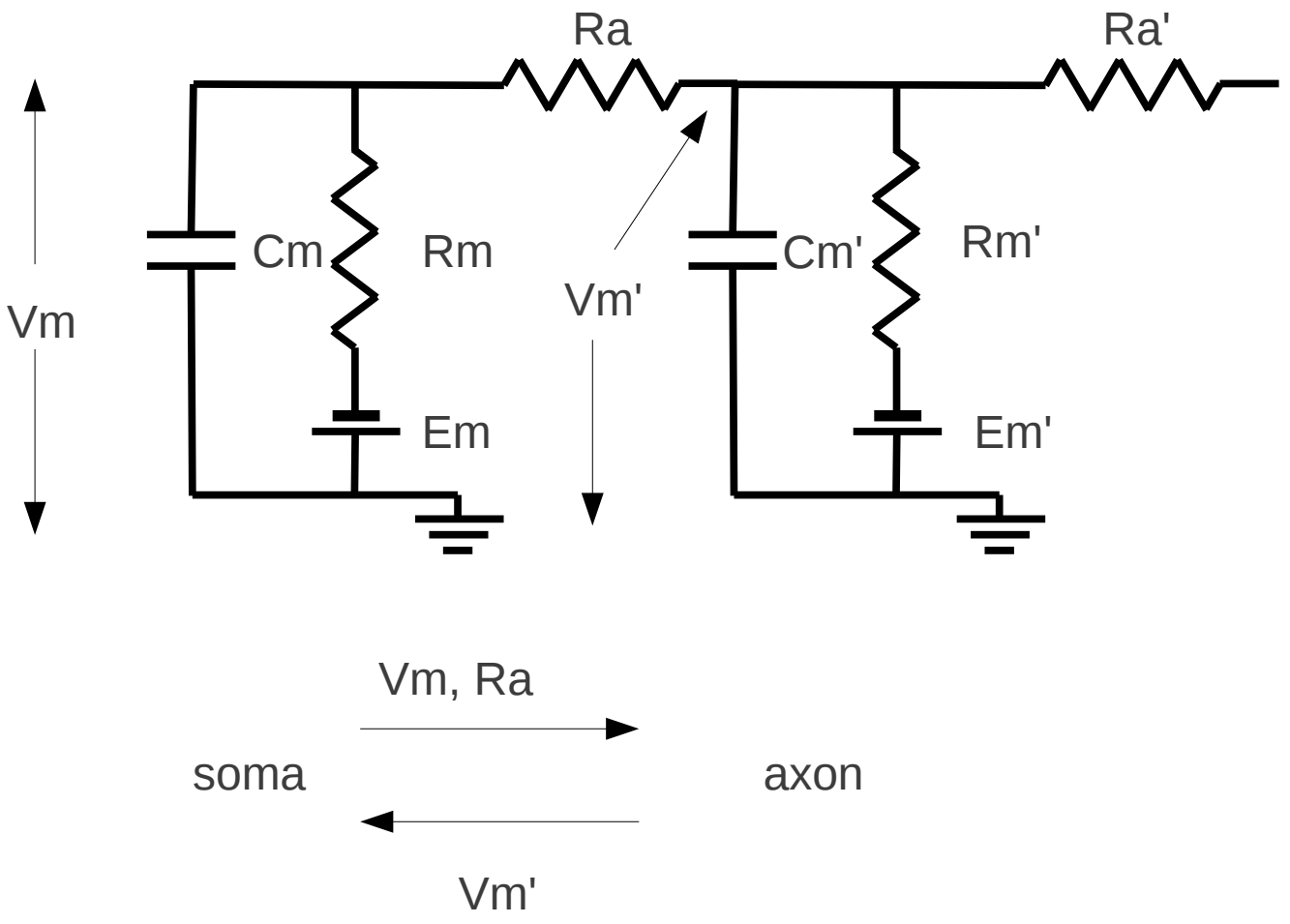
Scheduling

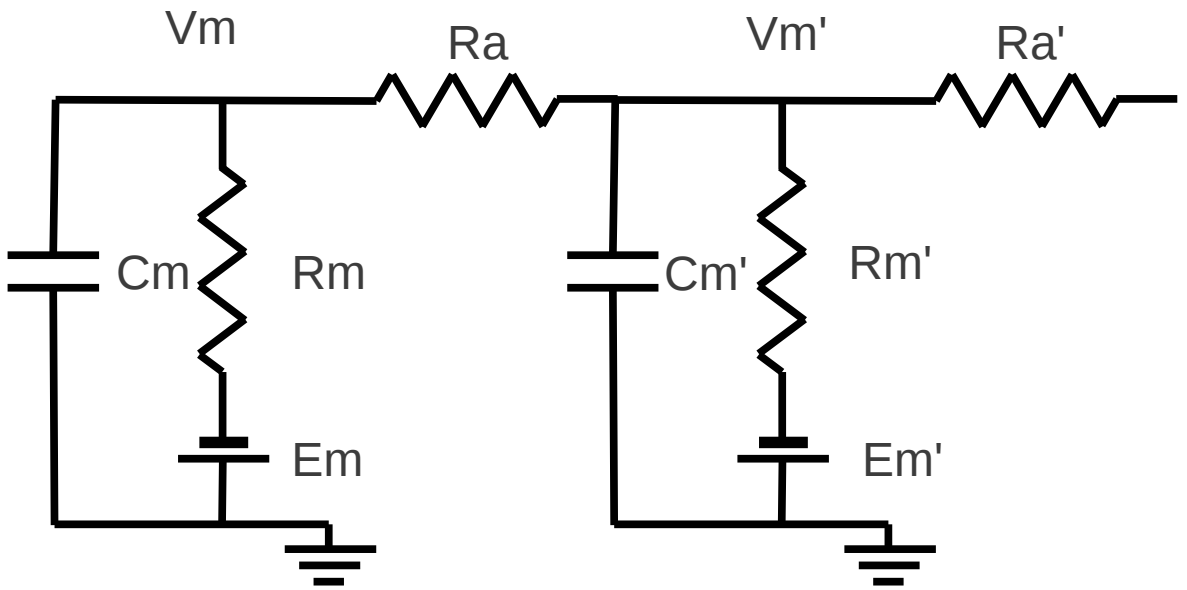
```
moose.context.setClock(0, sim_dt)
moose.context.setClock(1, sim_dt)
moose.context.setClock(2, plot_dt)

moose.context.useClock(0, '/soma',
'init')
moose.context.useClock(1,
'/##[TYPE=Compartment]',
'process')
moose.context.useClock(2, '/vm')
```

Running the simulation

```
moose.context.reset()


moose.context.step(50e-3)

vm_table.dumpFile('soma_vm.txt')
```

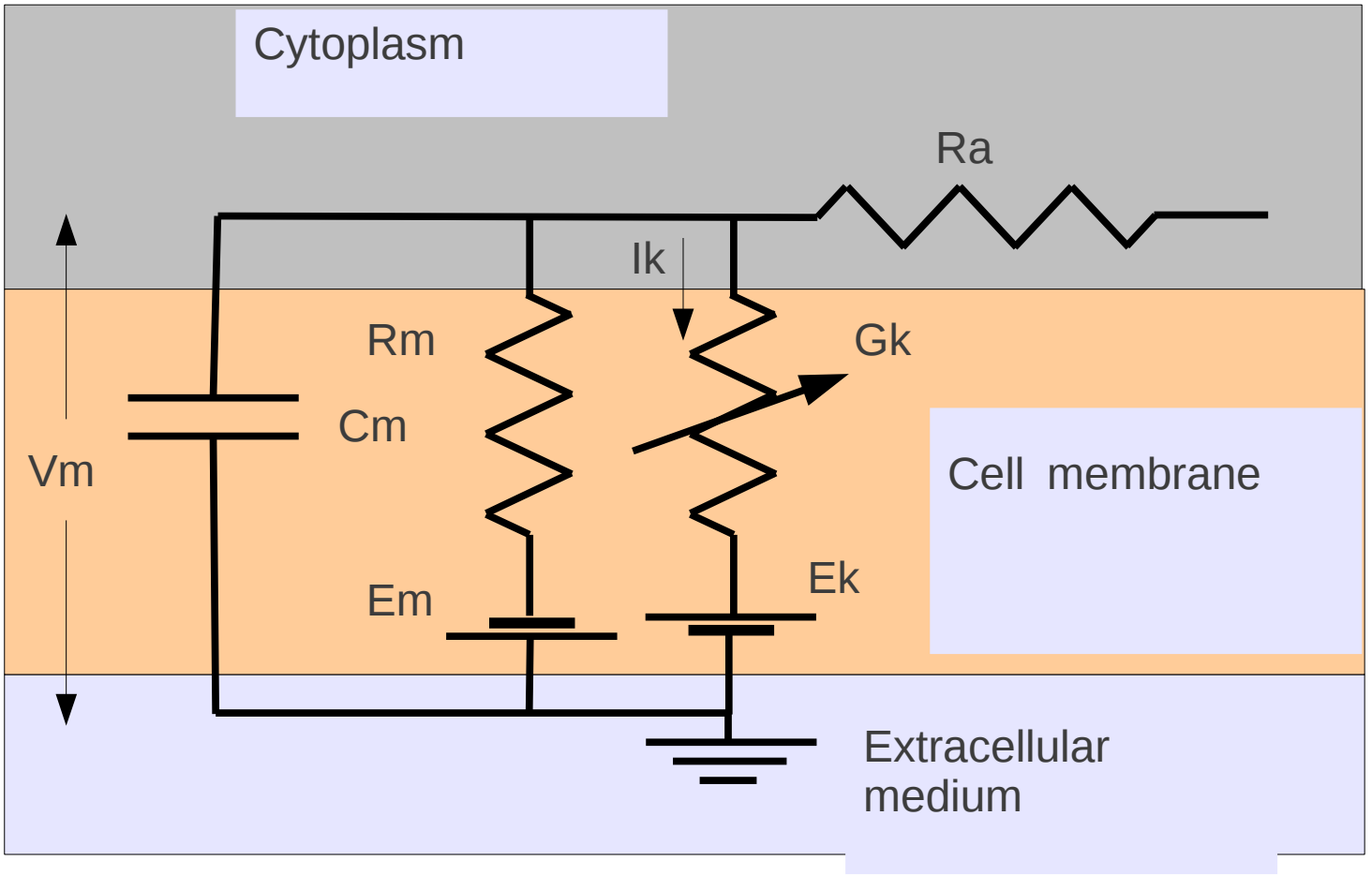
Adding another compartment






```
soma.Ra = 1e6
axon = moose.Compartment('axon')
…
soma.connect('raxial', axon, 'axial')
```

Inserting Hodgkin-Huxley-type ion channels



Setting up the channel

$$Gk = Gbar * m^3 * h$$

```
na_chan = moose.HHChannel('/soma/Na')
na_chan.Gbar = 1e-9
na_chan.Xpower = 3
na_chan.Ypower = 1
na_chan.connect('channel', soma,
'channel')
```

Setting up the gates

$$\frac{dm}{dt} = alpha * (1 - m) - beta * m$$

$$alpha = \frac{A + B * Vm}{C + \exp\left(\frac{D + Vm}{F}\right)}$$

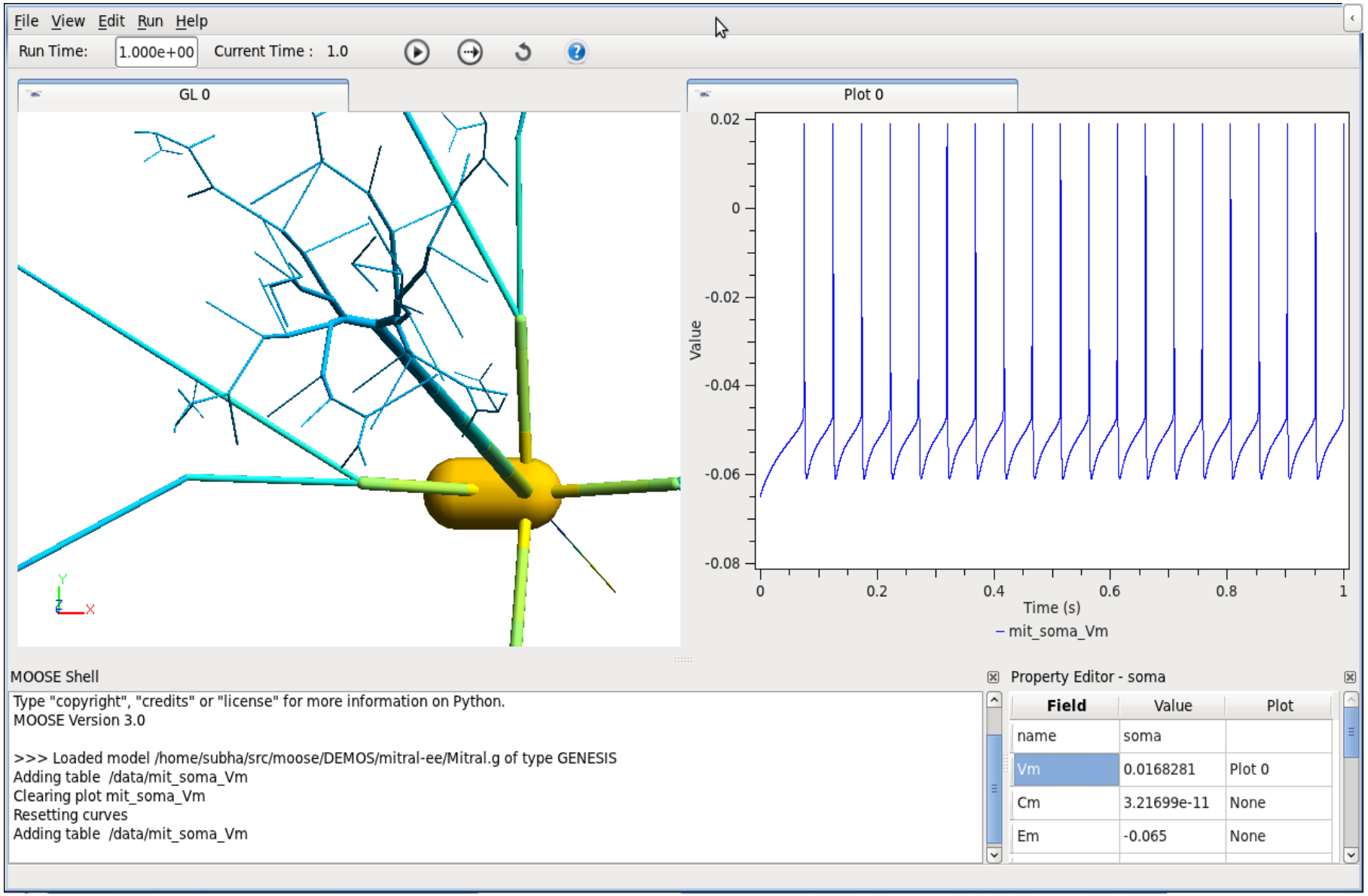
Equation for *beta* has same form as *alpha*

```
na_chan.setupAlpha('xGate',
    alphaA,alphaB,alphaC,alphaD,alphaF,
     betaA,betaB,betaC,betaD,betaF,
                          divs,vmin,vmax)
```

Or simply ...

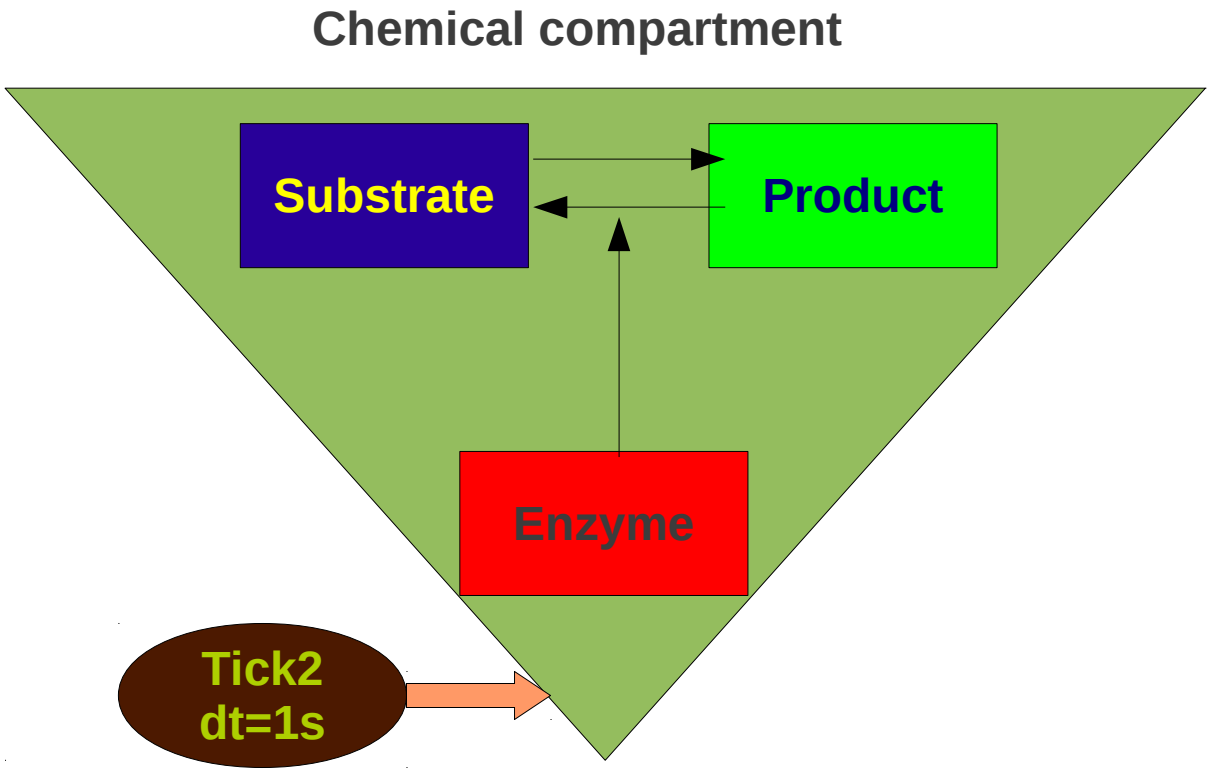
```
from moose import neuroml
reader = neuroml.NeuroML()

reader.readNeuroMLFromFile(
    'GranuleGenerated.net.xml')

cell = moose.Cell('/Gran_0')
```

Even simpler: use MOOSE GUI



Multiscale modeling

- Ticks with different time-steps run different components of a model at different rates.



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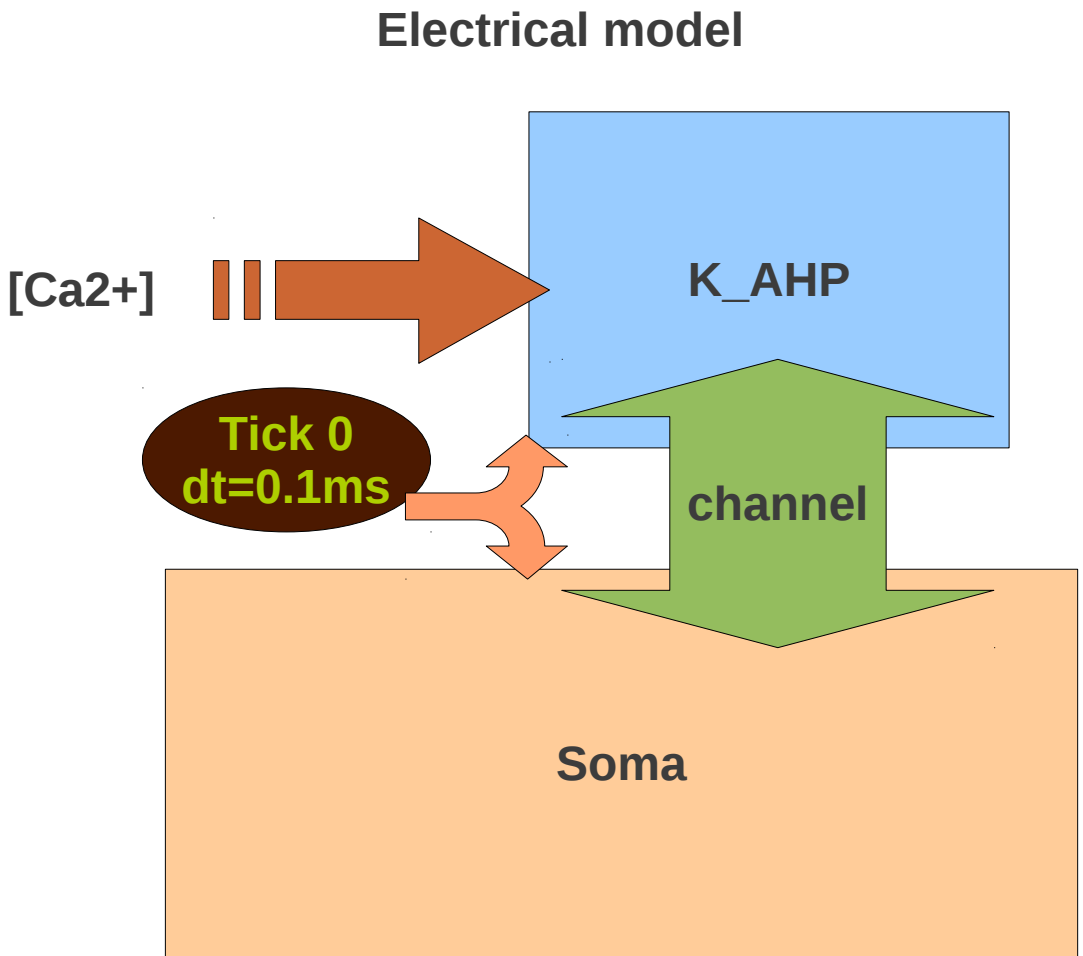

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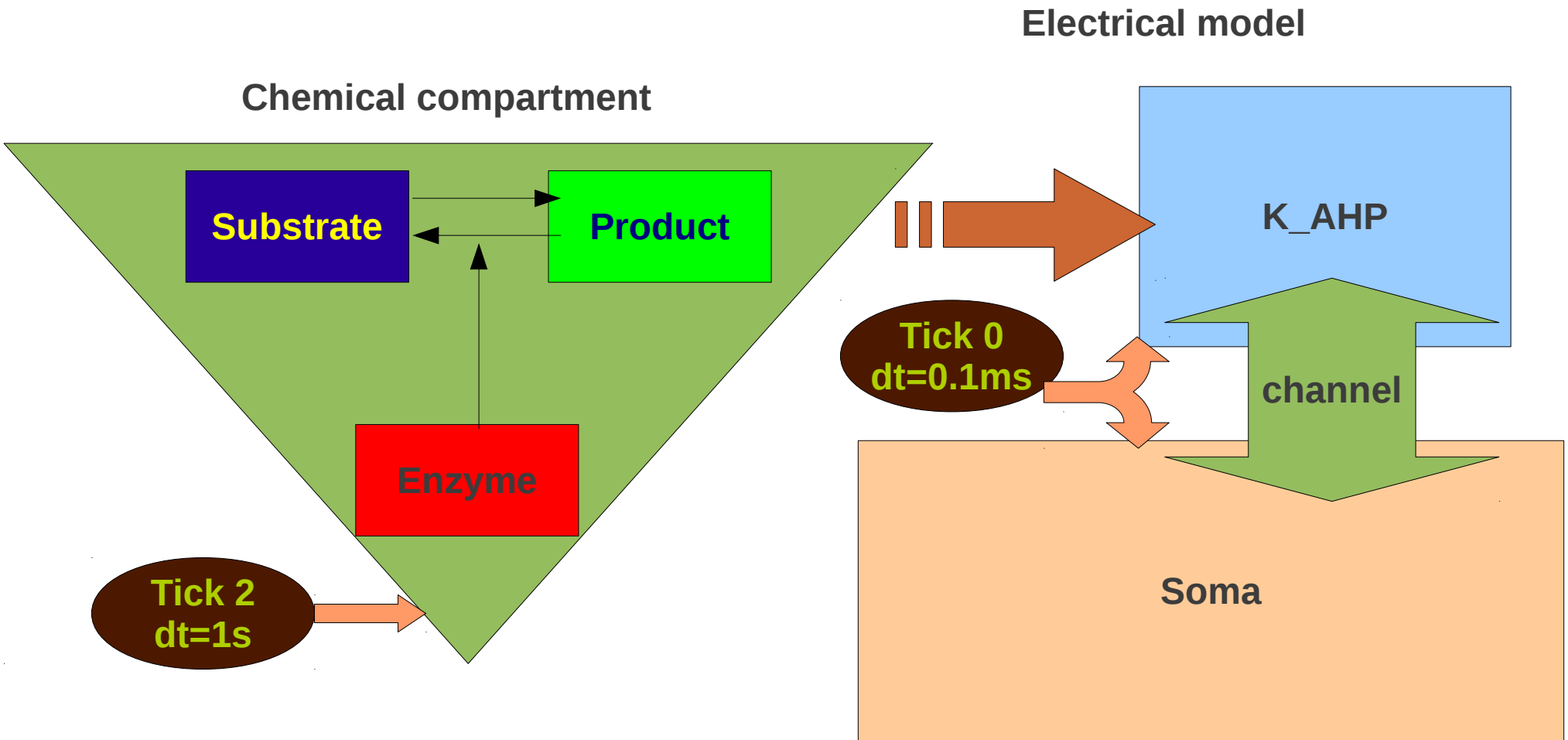

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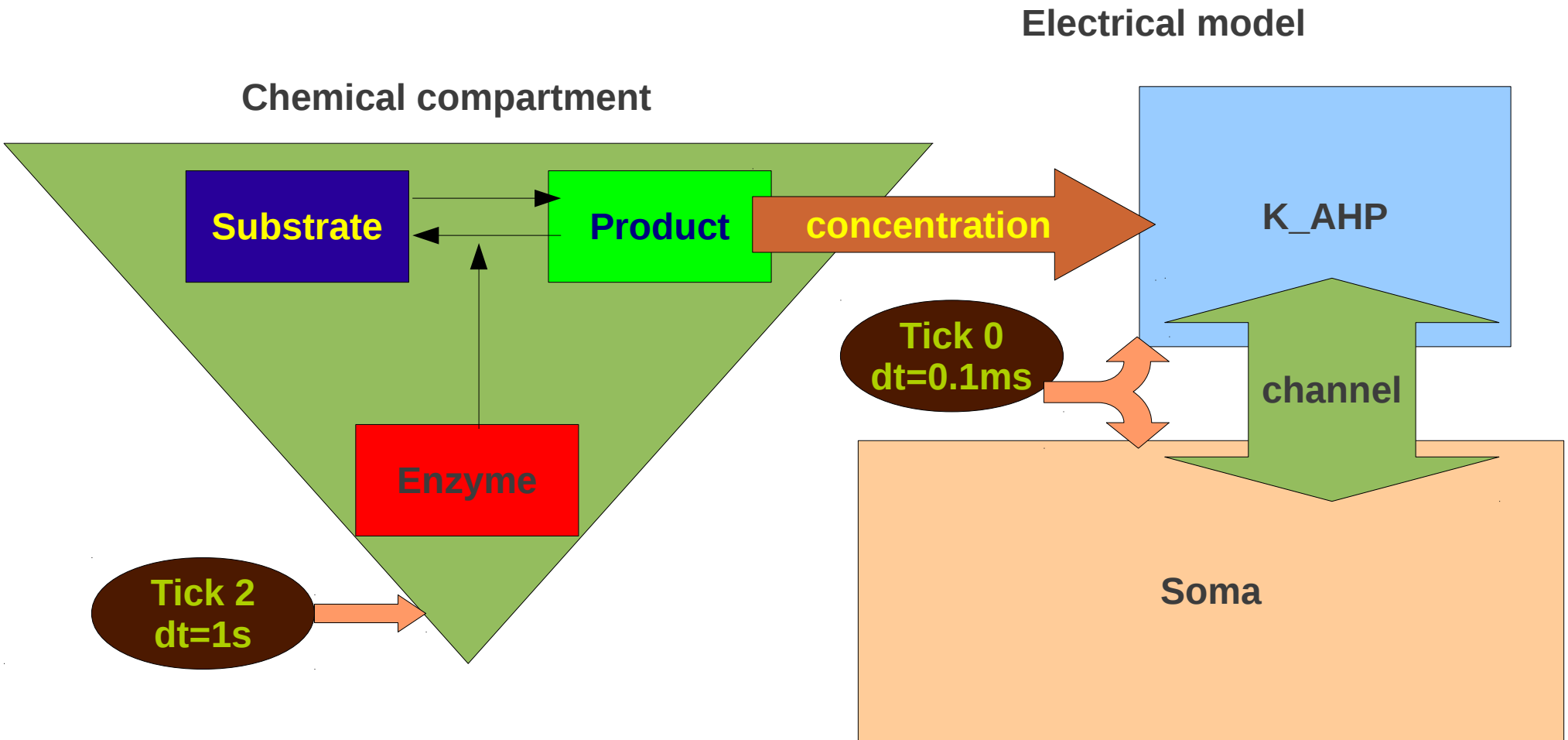
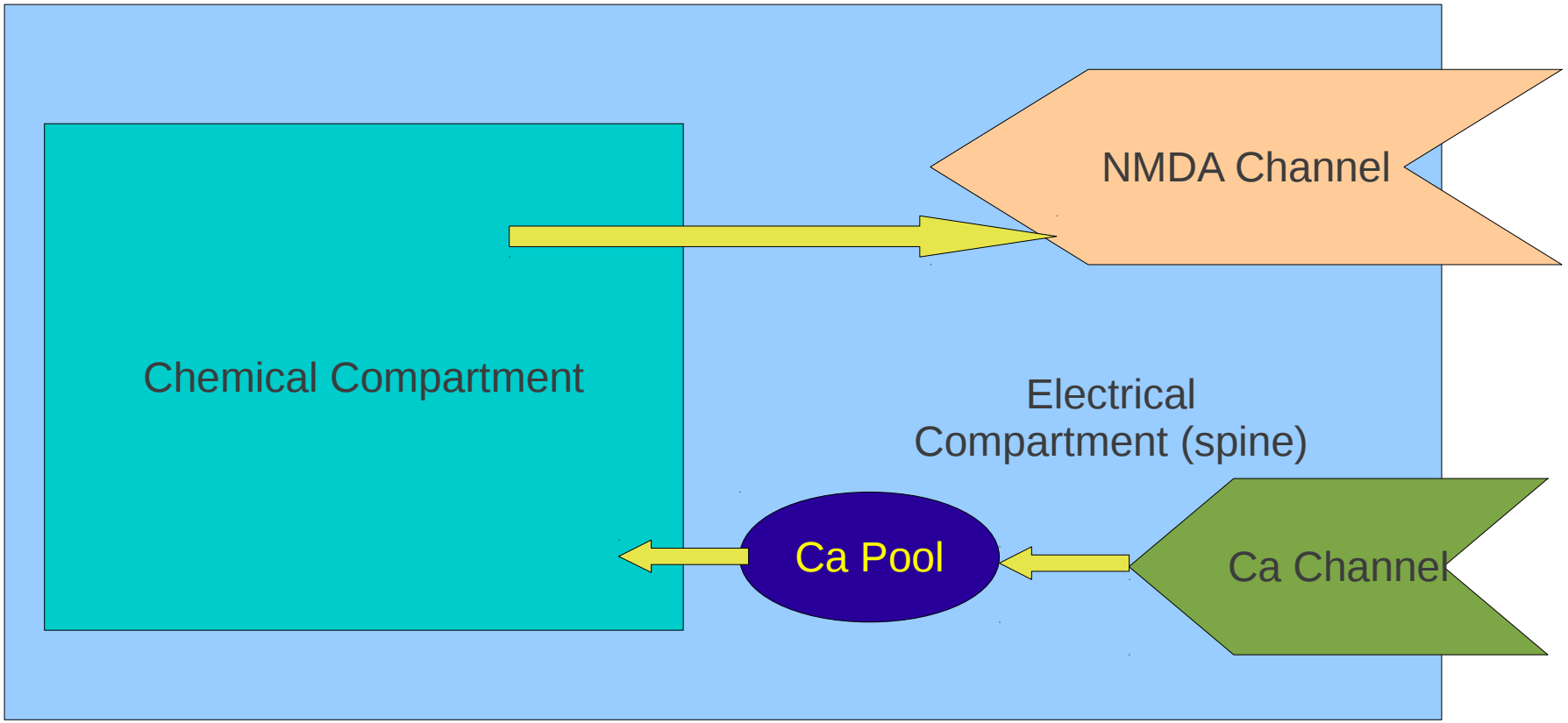
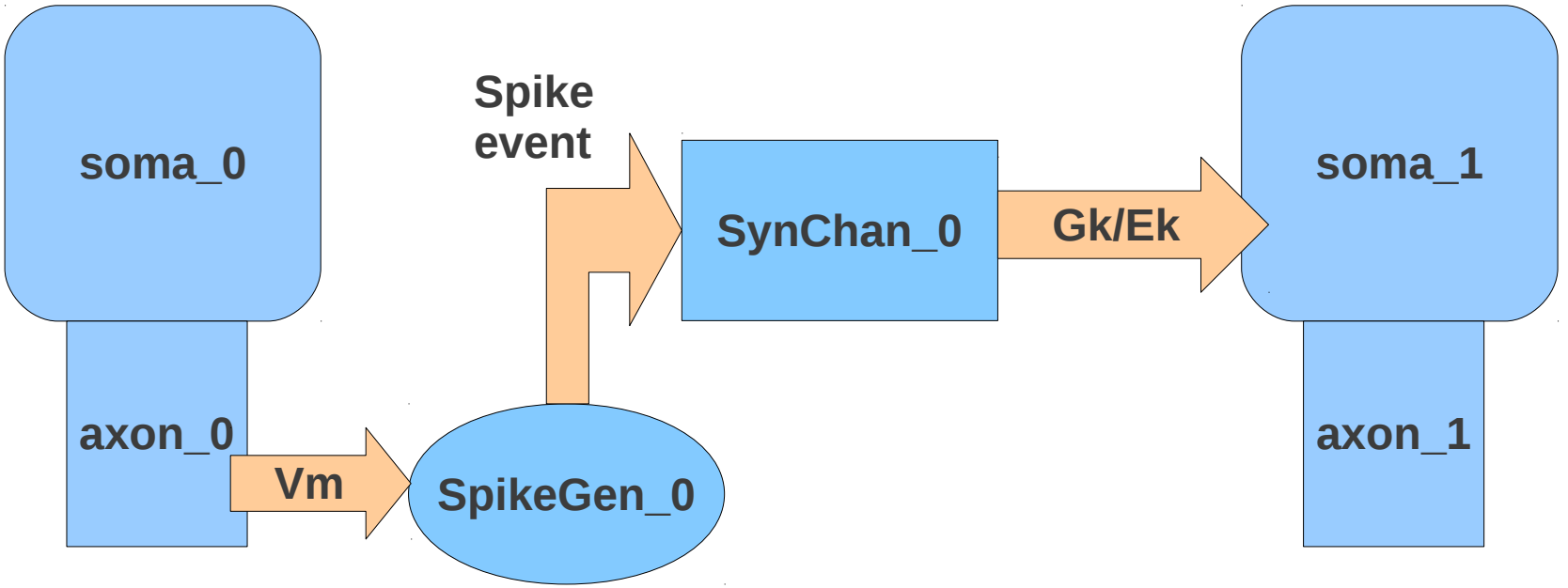


A more realistic system



Multiscale modeling: networks

- You can connect neuronal compartments via synapse to create a network.



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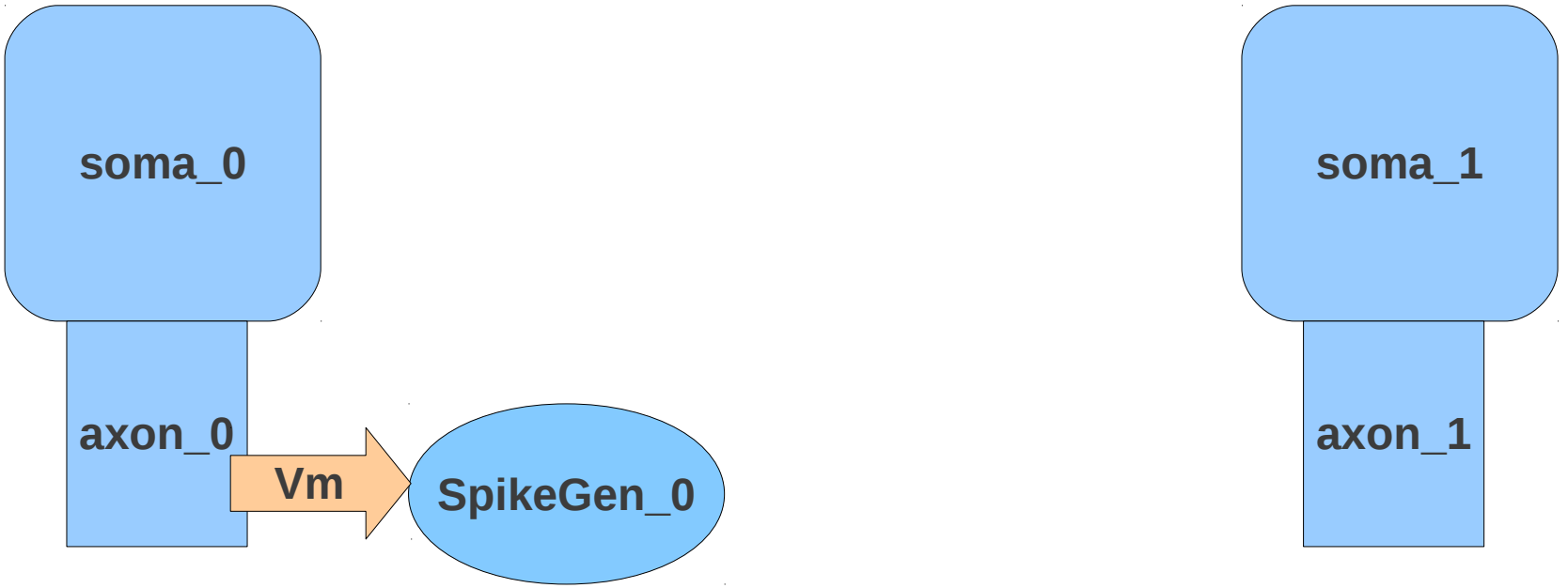

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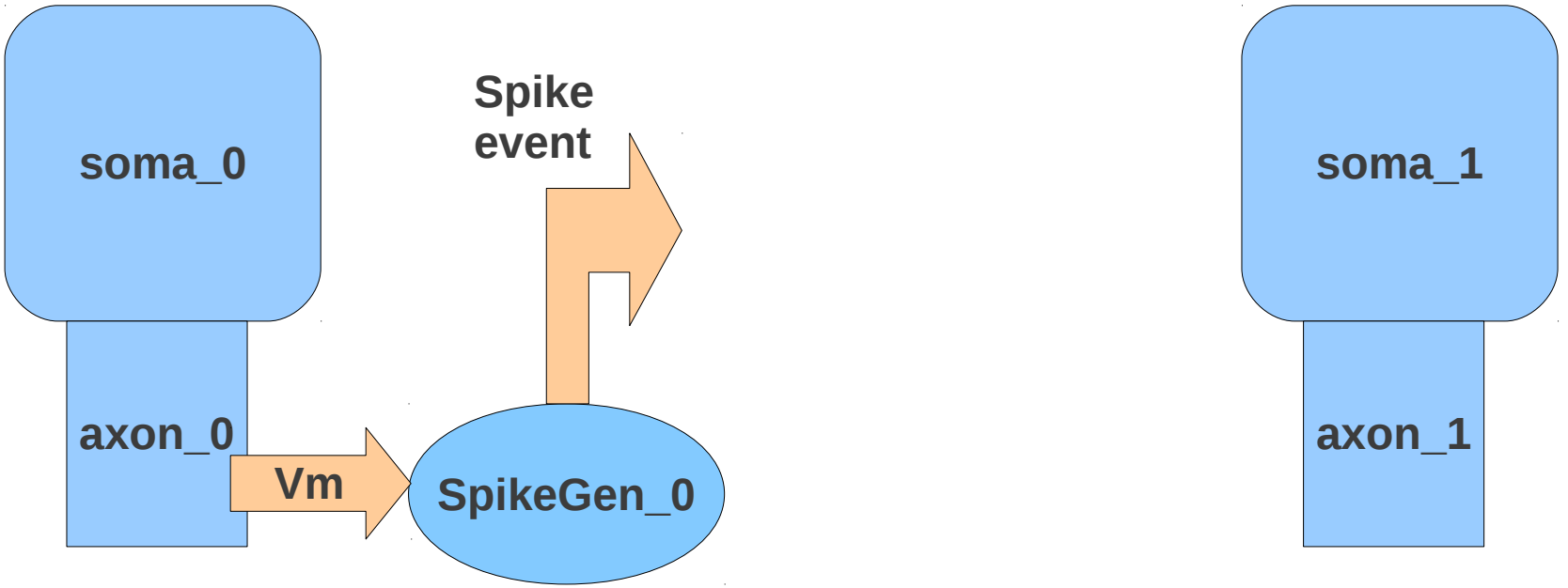

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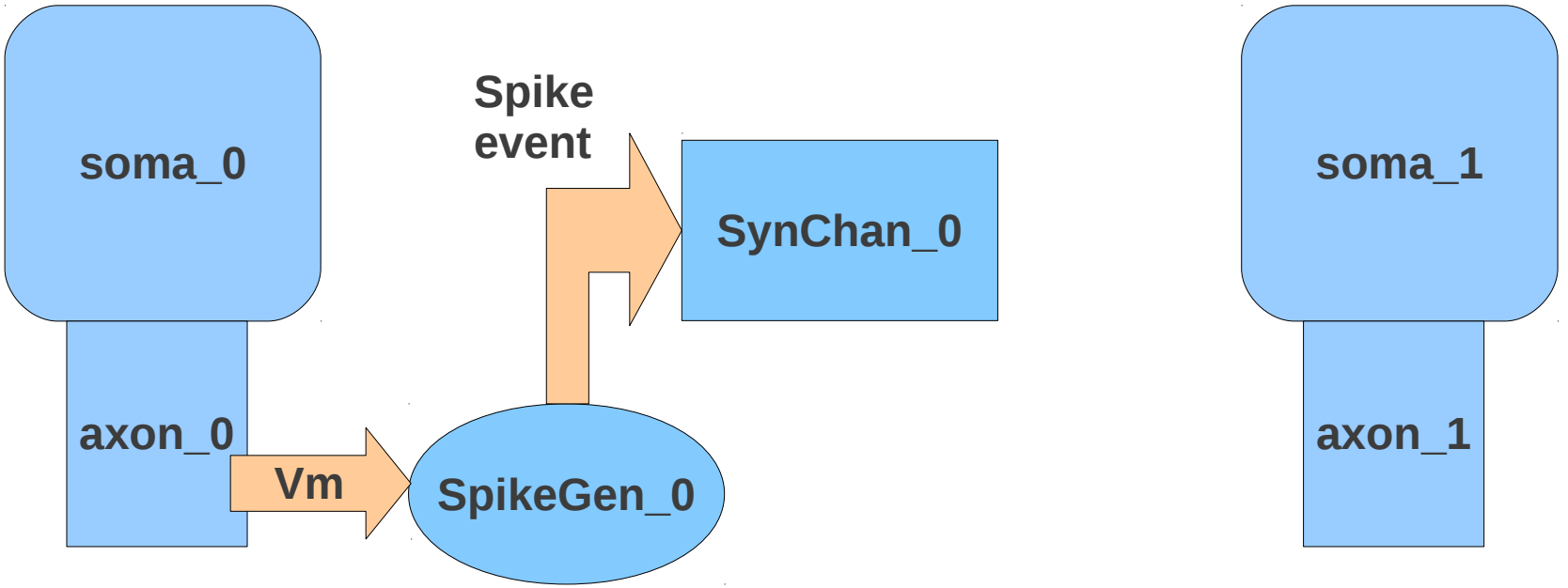

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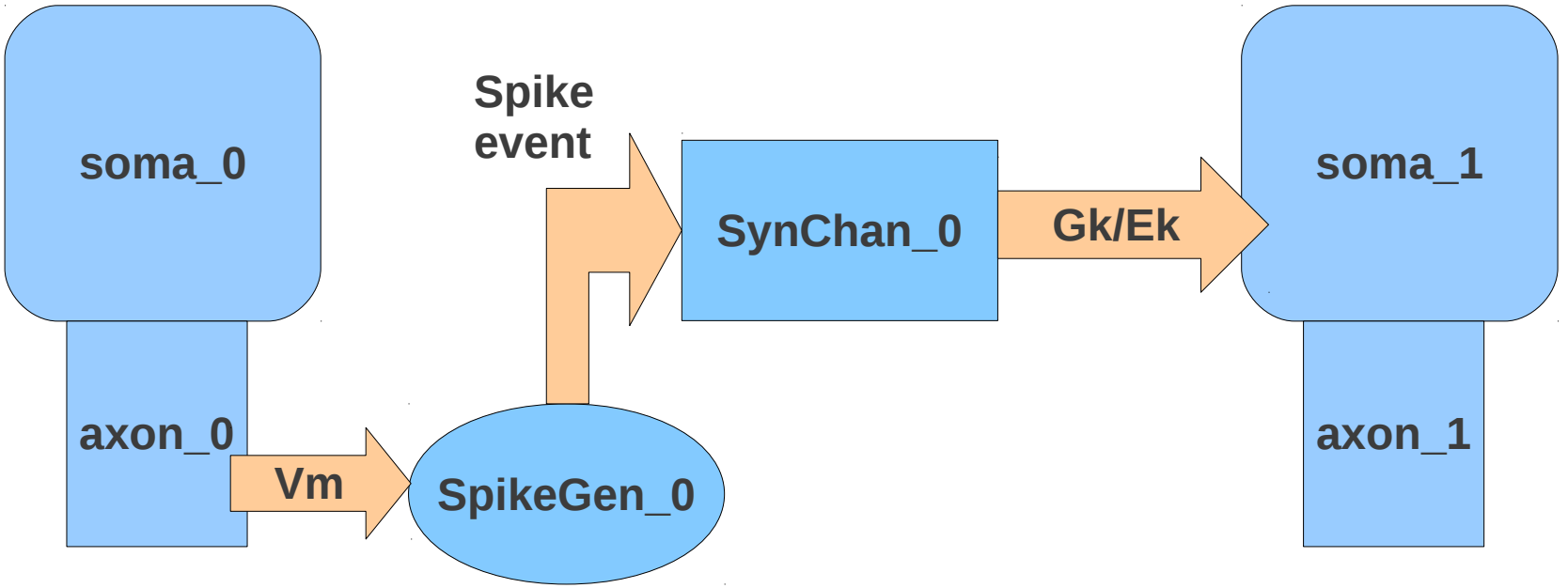
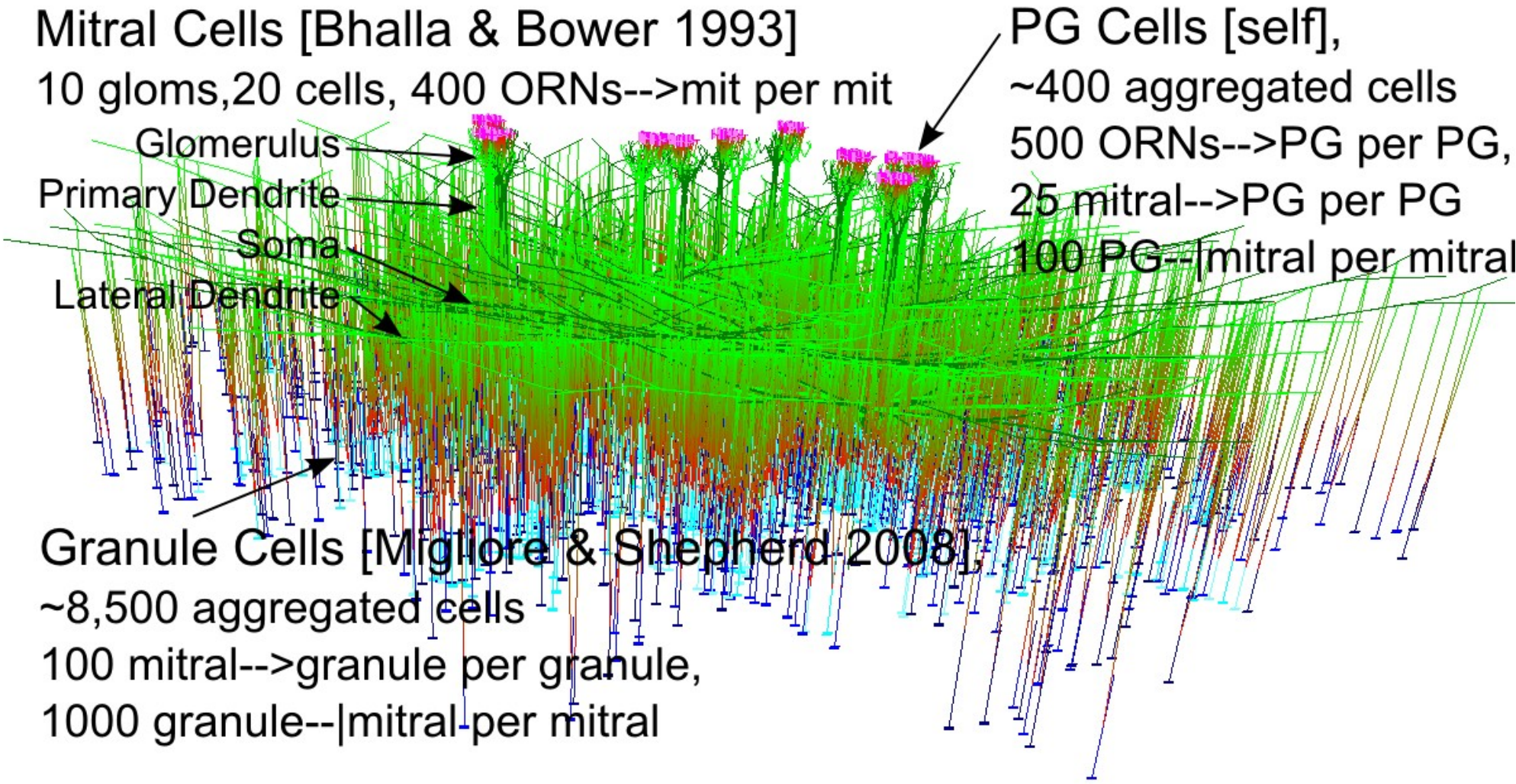
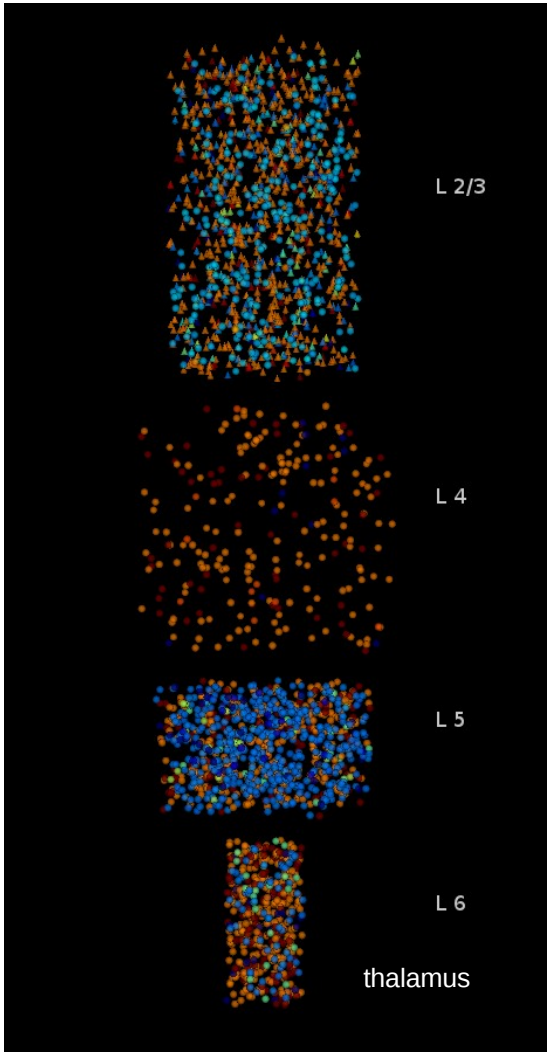


Multiscale modeling: Olfactory bulb

Aditya Gilra



Multiscale modeling: Cortical column



- Detailed biophysical model of single thalamocortical column (based on Traub et al 2005) of rat barrel cortex:

  14 cell types

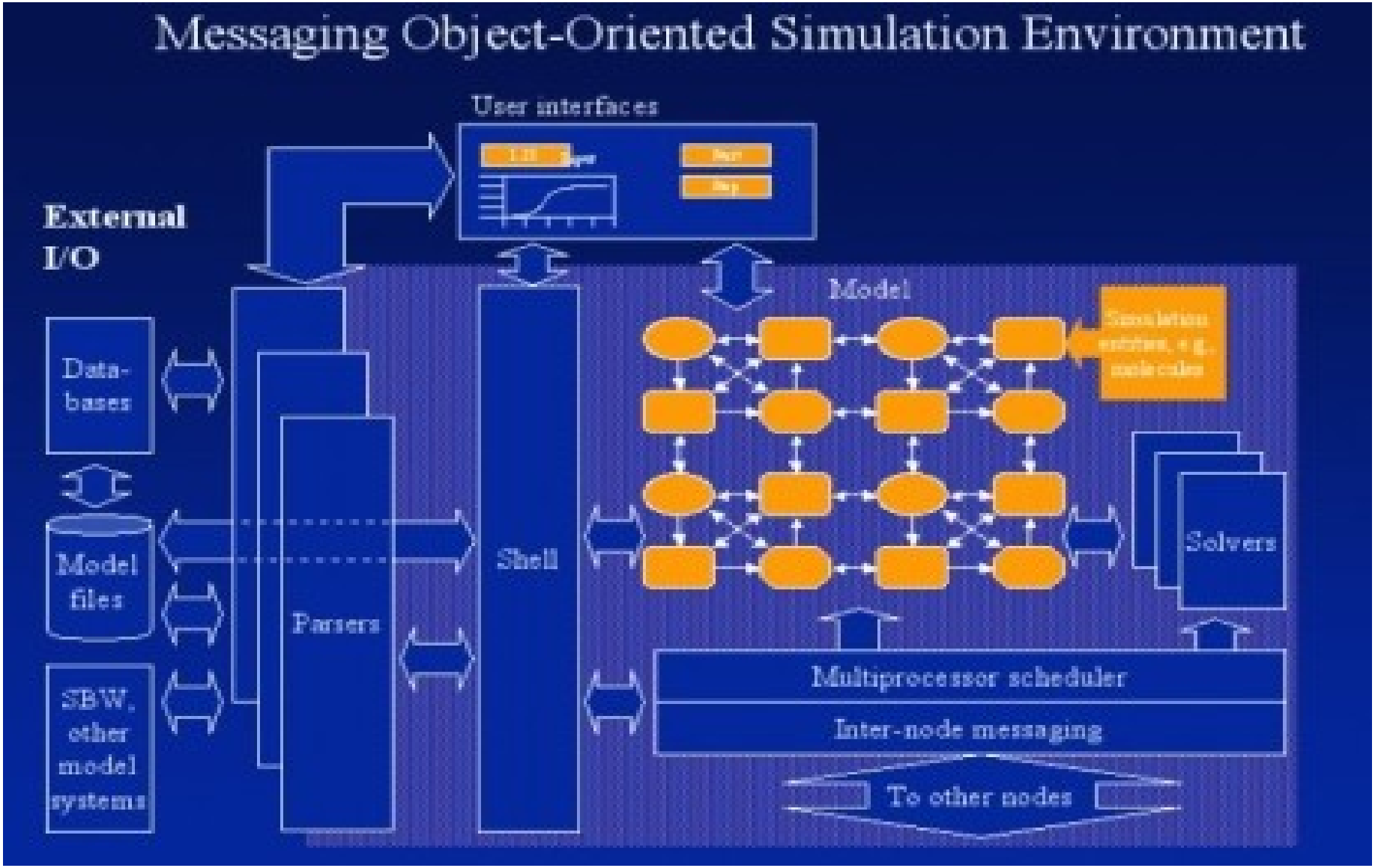
  50-120 compartments

  11 ion channel types

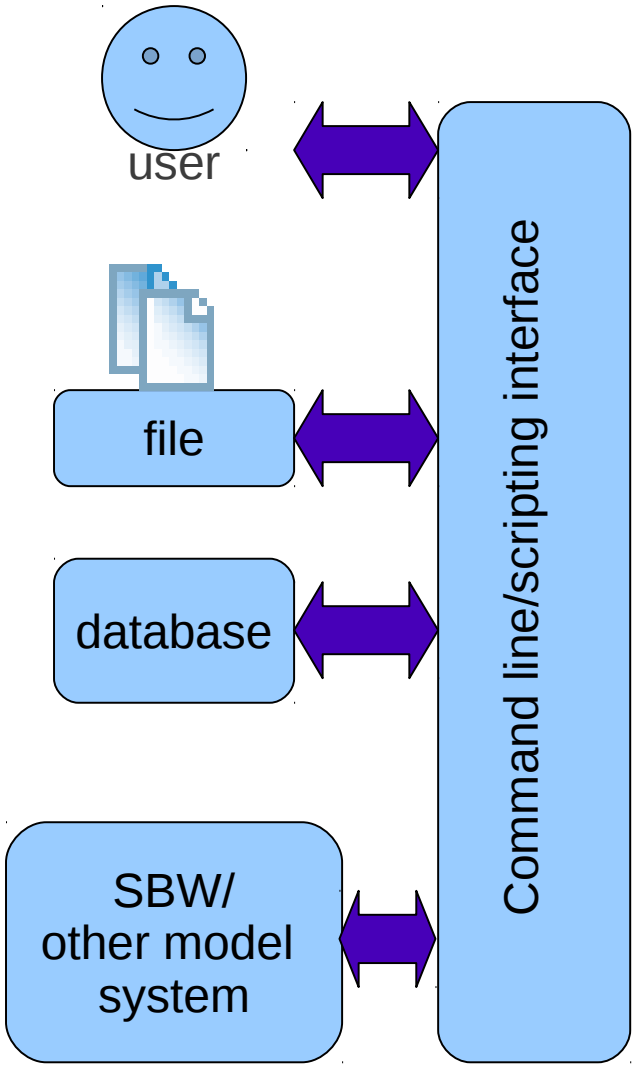
  ~3500 cells

MOOSE Architecture

Figure: Upi Bhalla



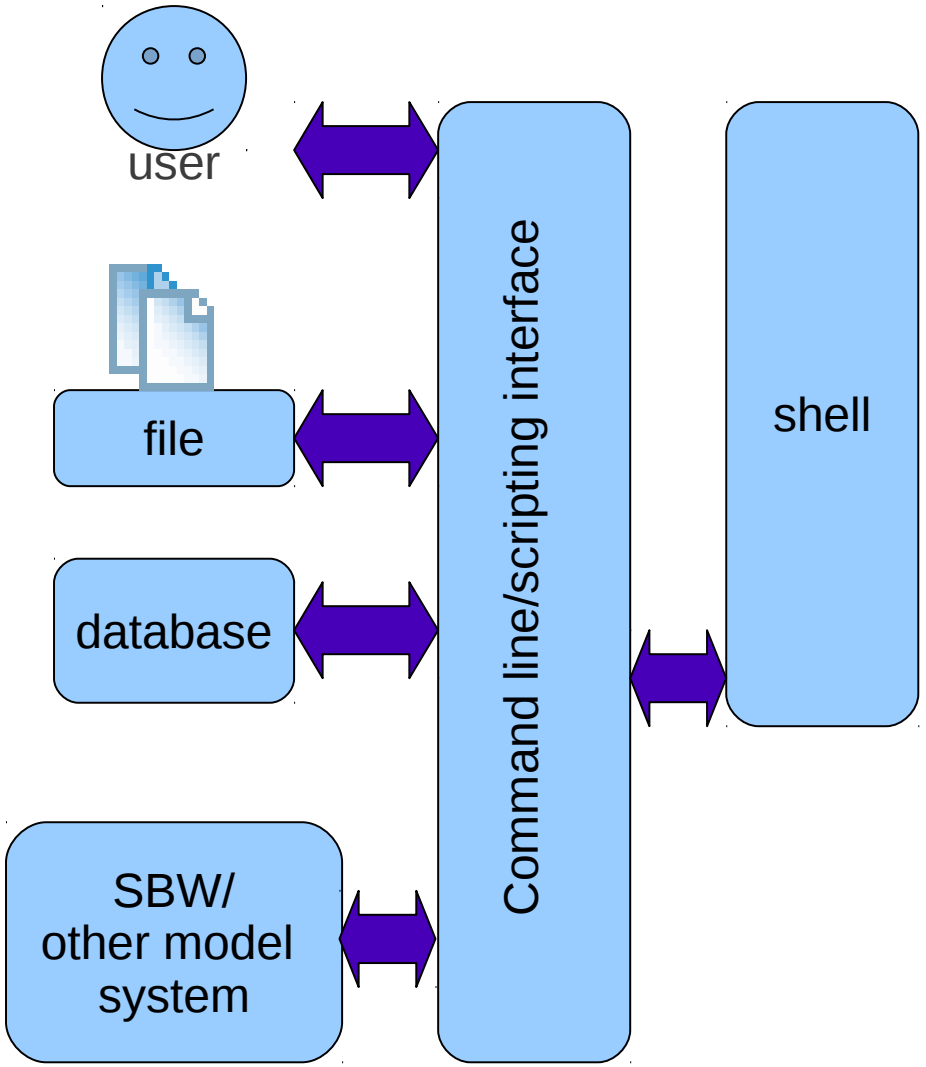
MOOSE Architecture: scripting interface



The command line / scripting interface is where modeler interacts with MOOSE.

Derived from:
http://moose.sourceforge.net/images/stories/architecture_65.jpg

MOOSE Architecture: Shell



The user interface talks to

Shell - the single point of access to all functionalities available to the user

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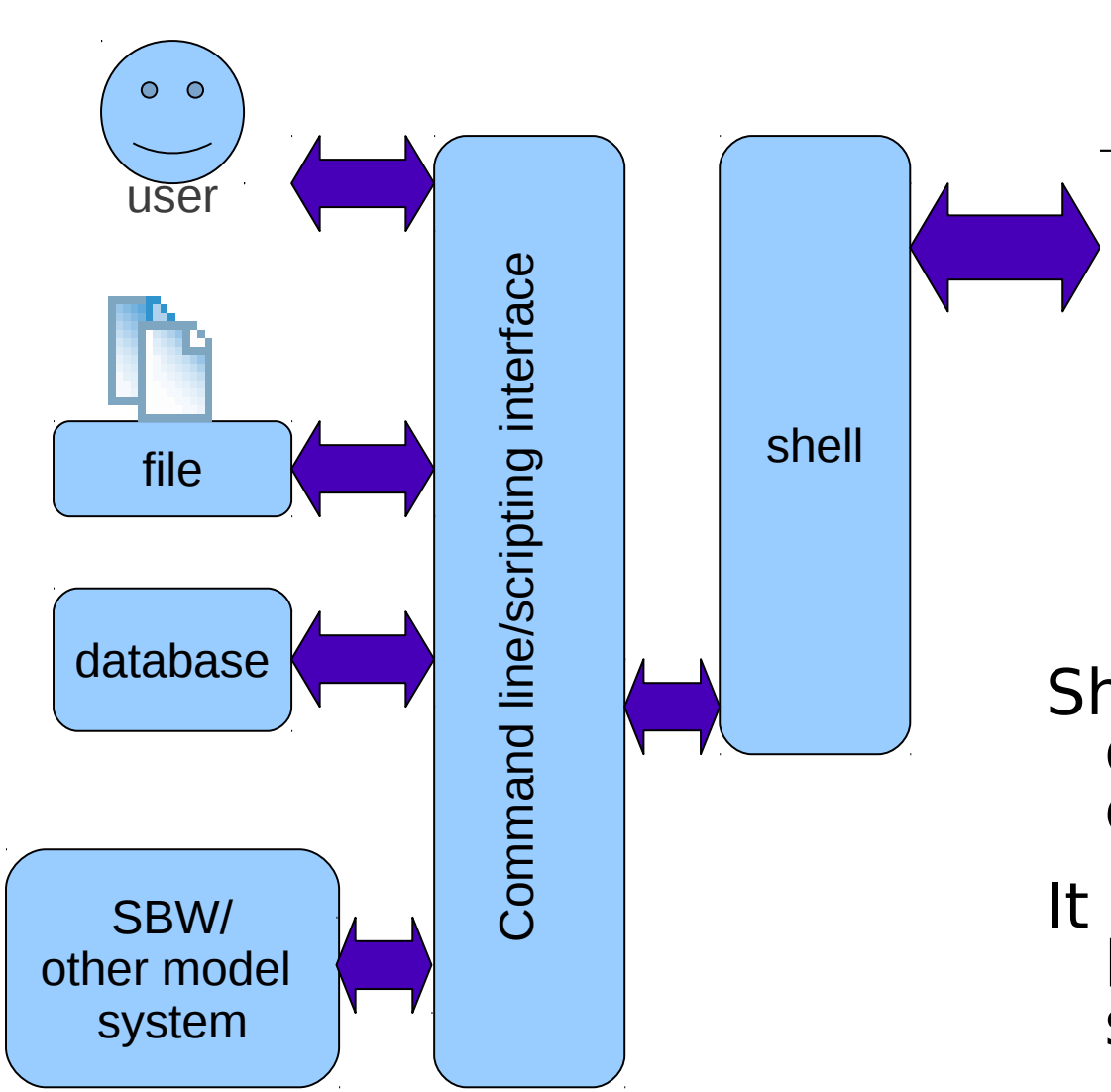
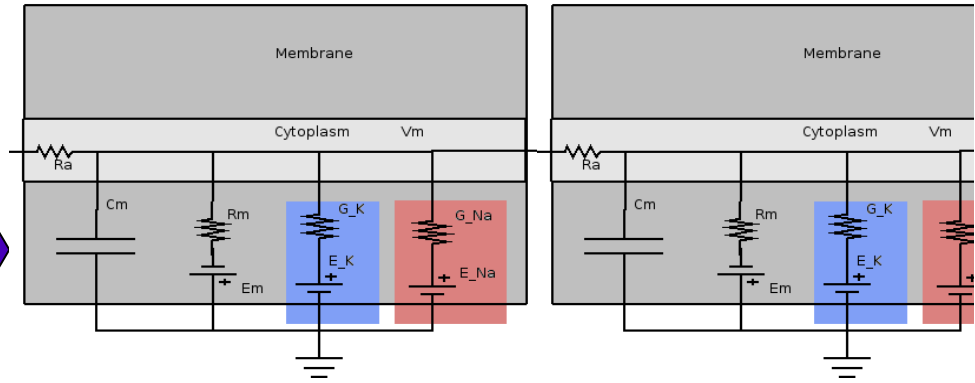
MOOSE Architecture





Simulation entities

Shell creates, deletes and queries other MOOSE objects.

It also executes some of the built-in functionalities reinit, start.

Derived from:
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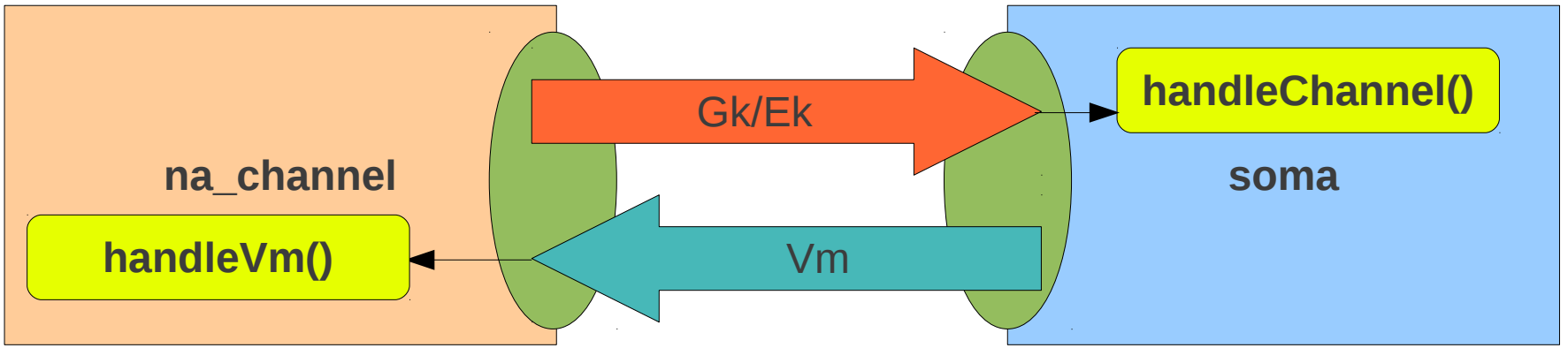
MOOSE Architecture: Messaging

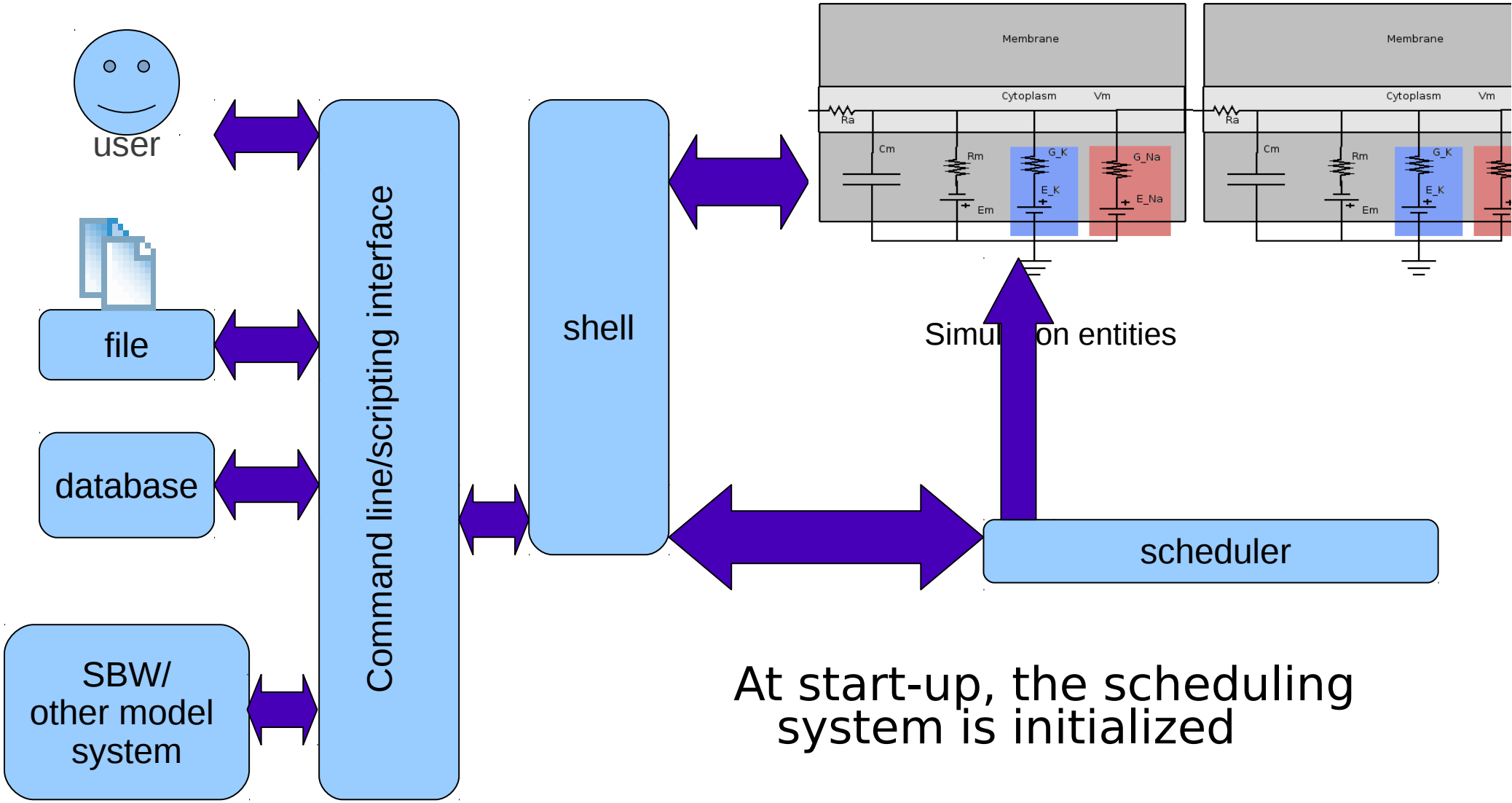
Objects communicate state variables during simulation.

Destination fields give handle to functions for callback.

```
na_channel.connect('channel',
                   soma, 'channel')
```



MOOSE Architecture: scheduling



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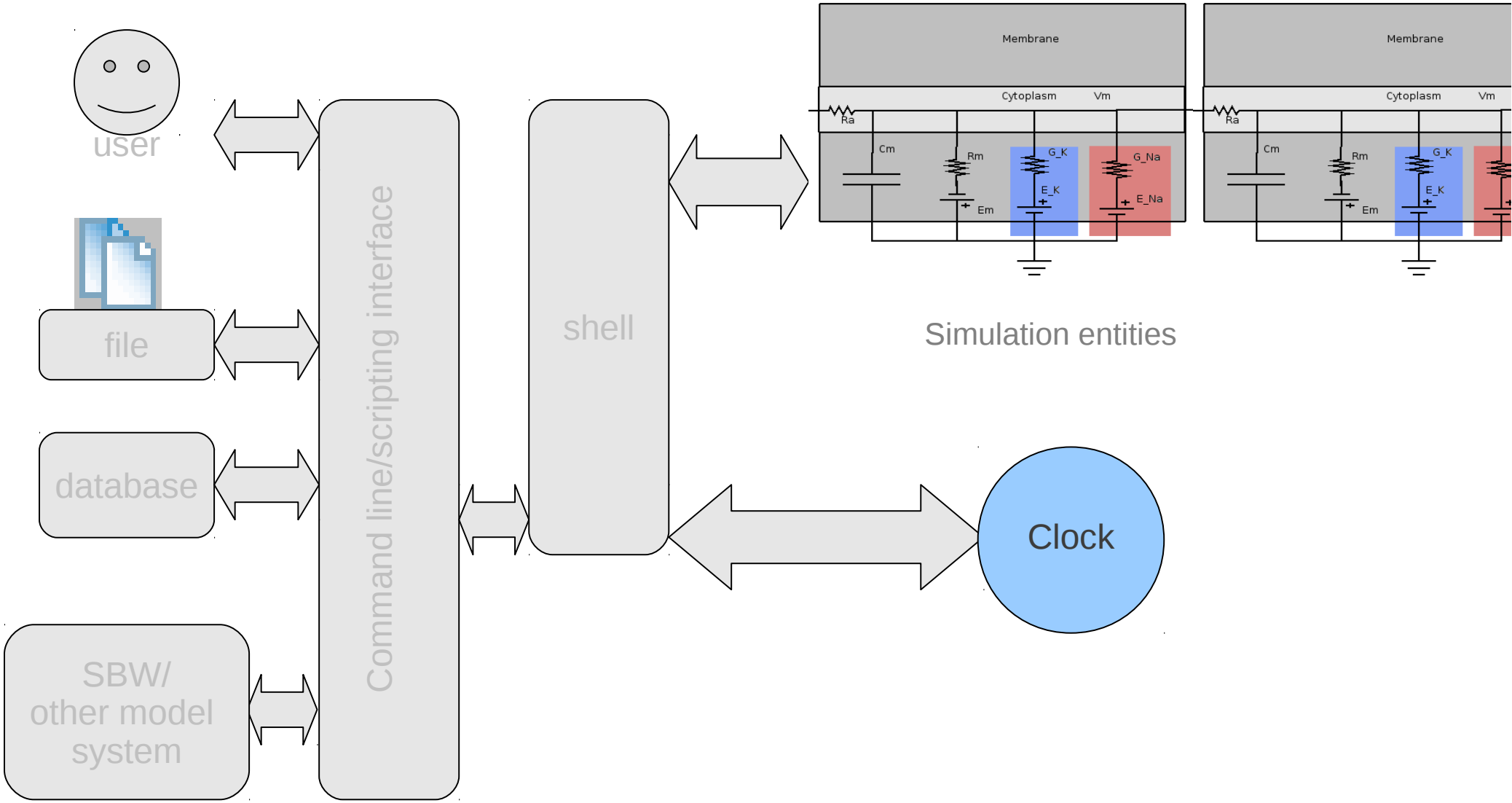

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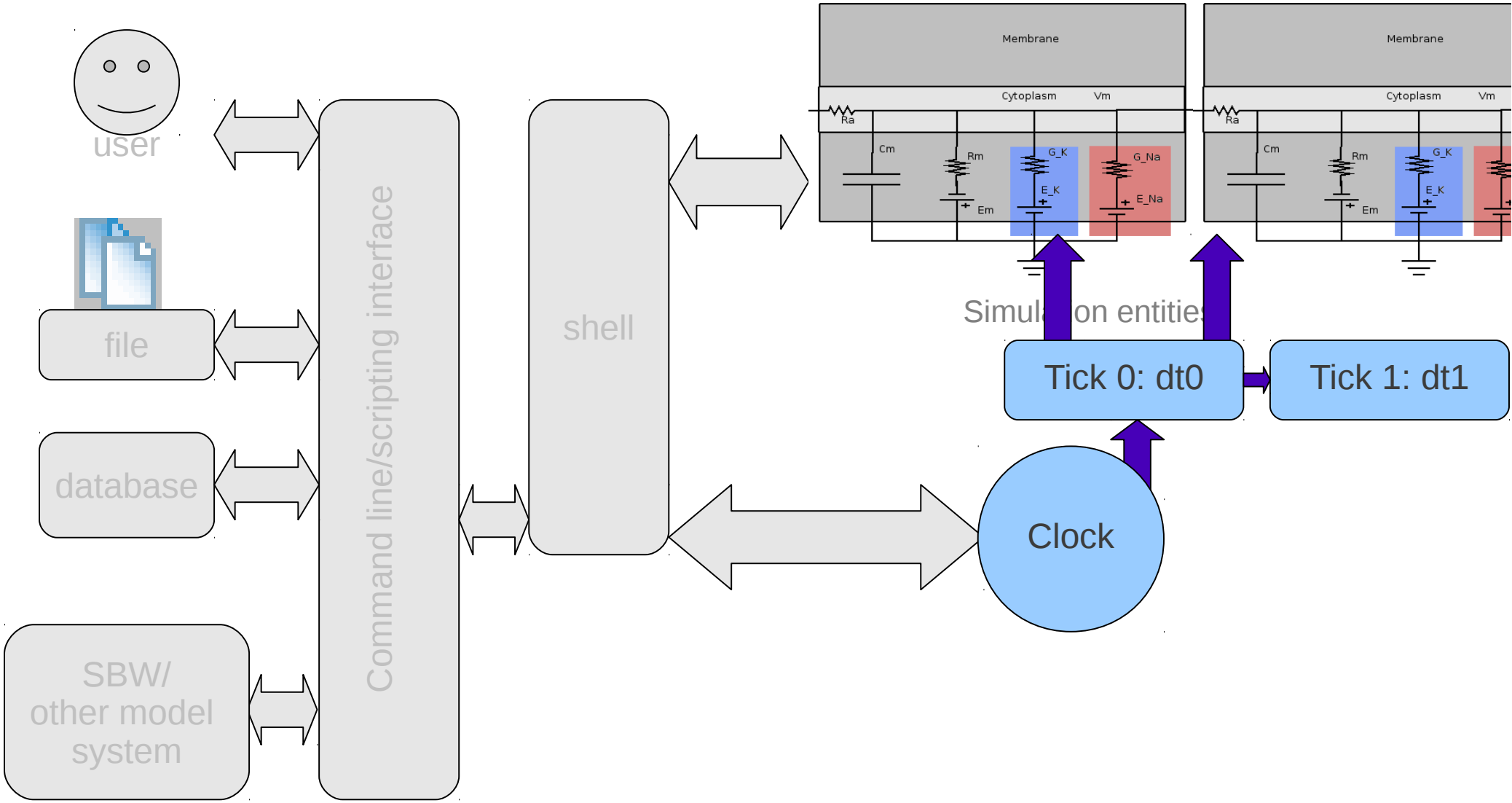

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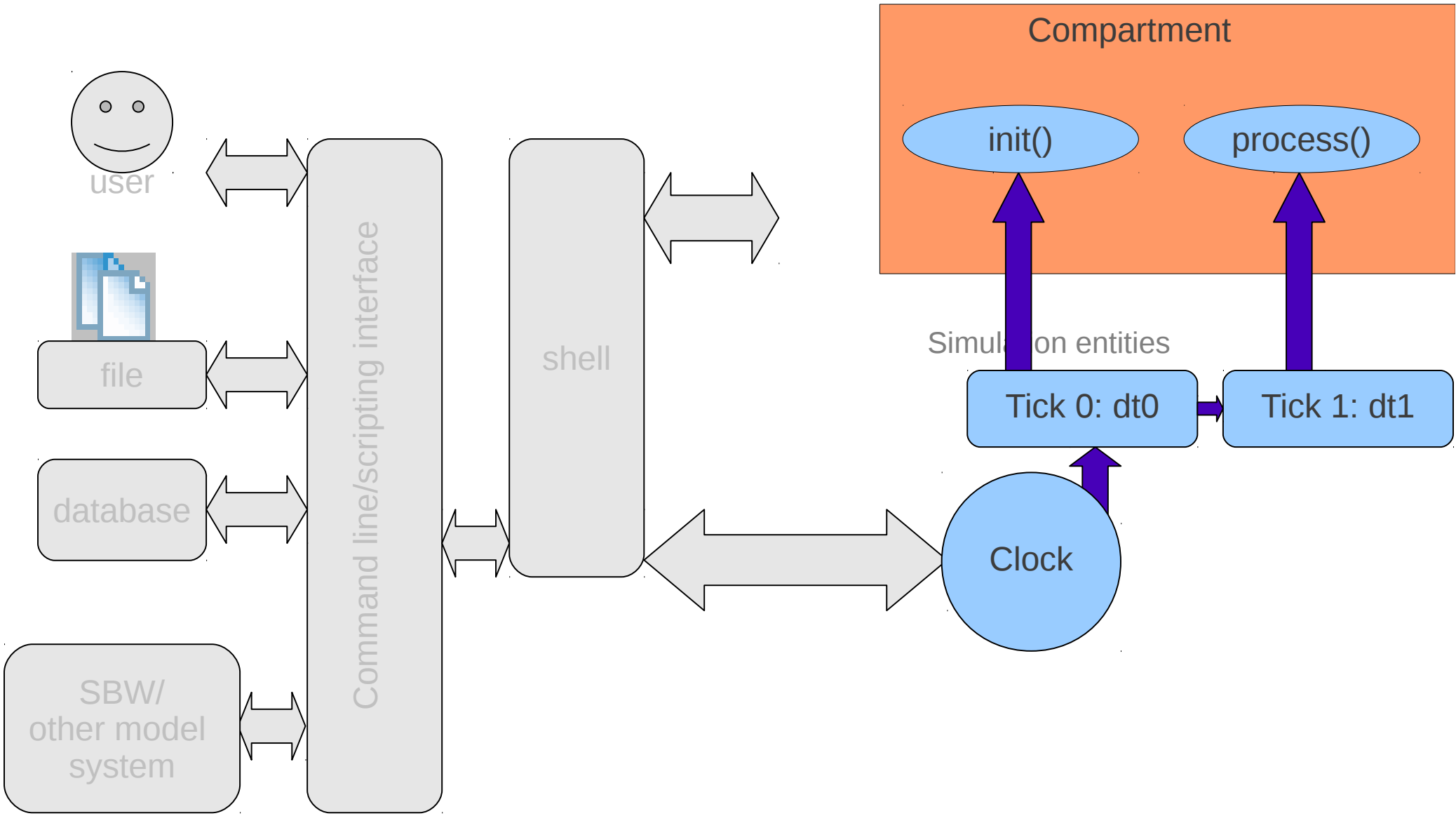

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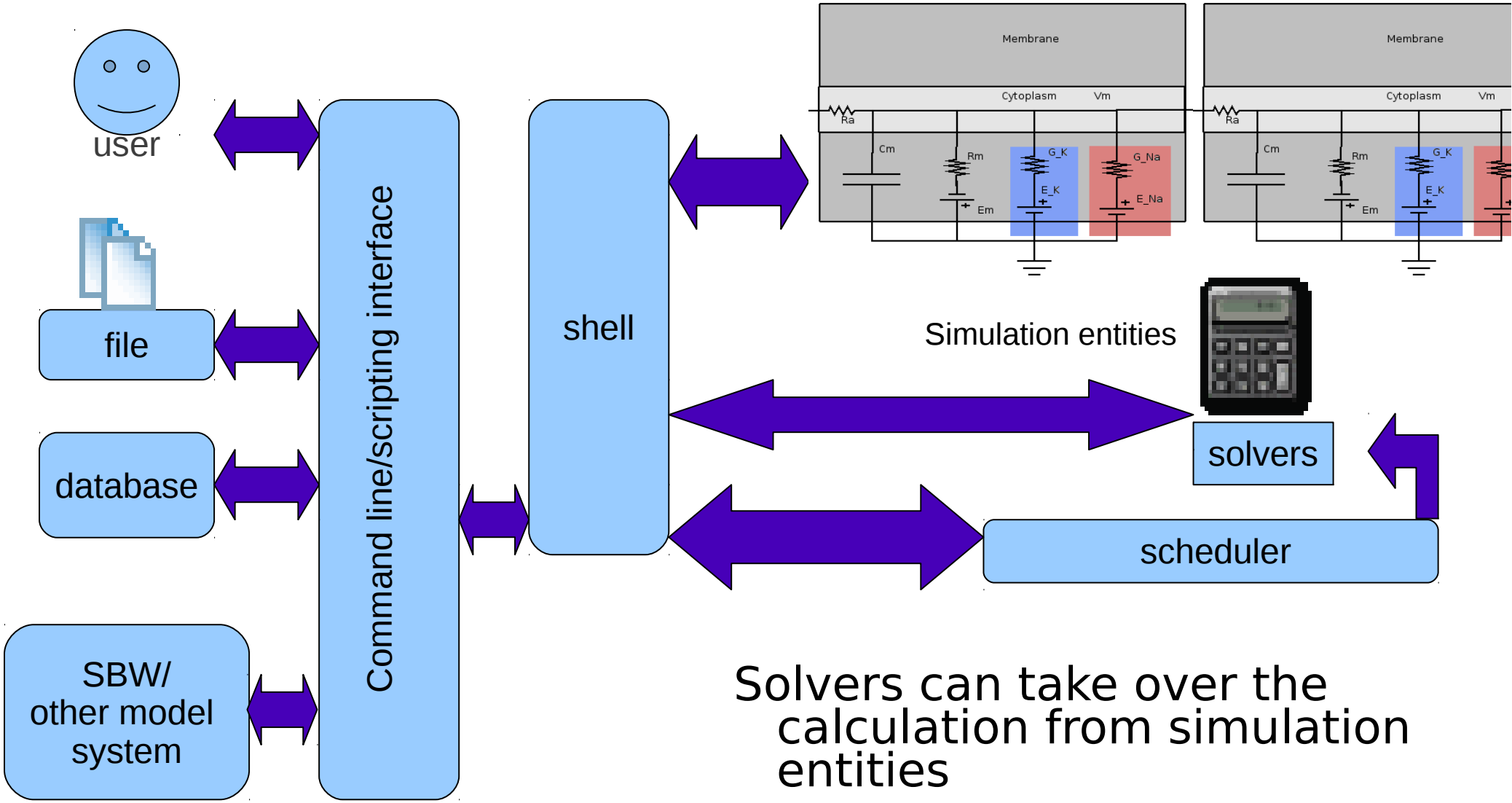
MOOSE Architecture: solvers



Solvers can take over the calculation from simulation entities

Derived from:
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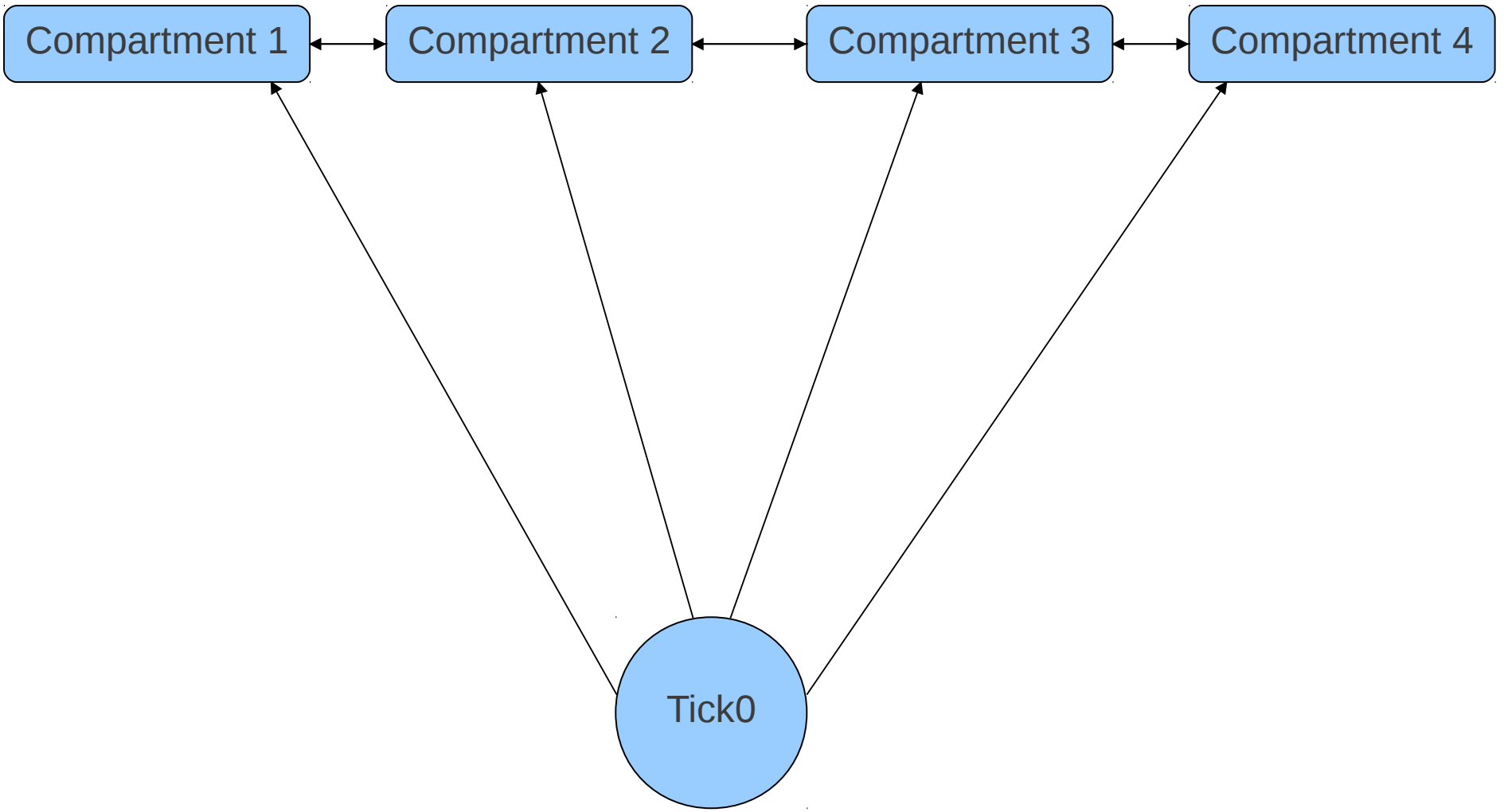
Solvers: Avoid the penalty of object orientation



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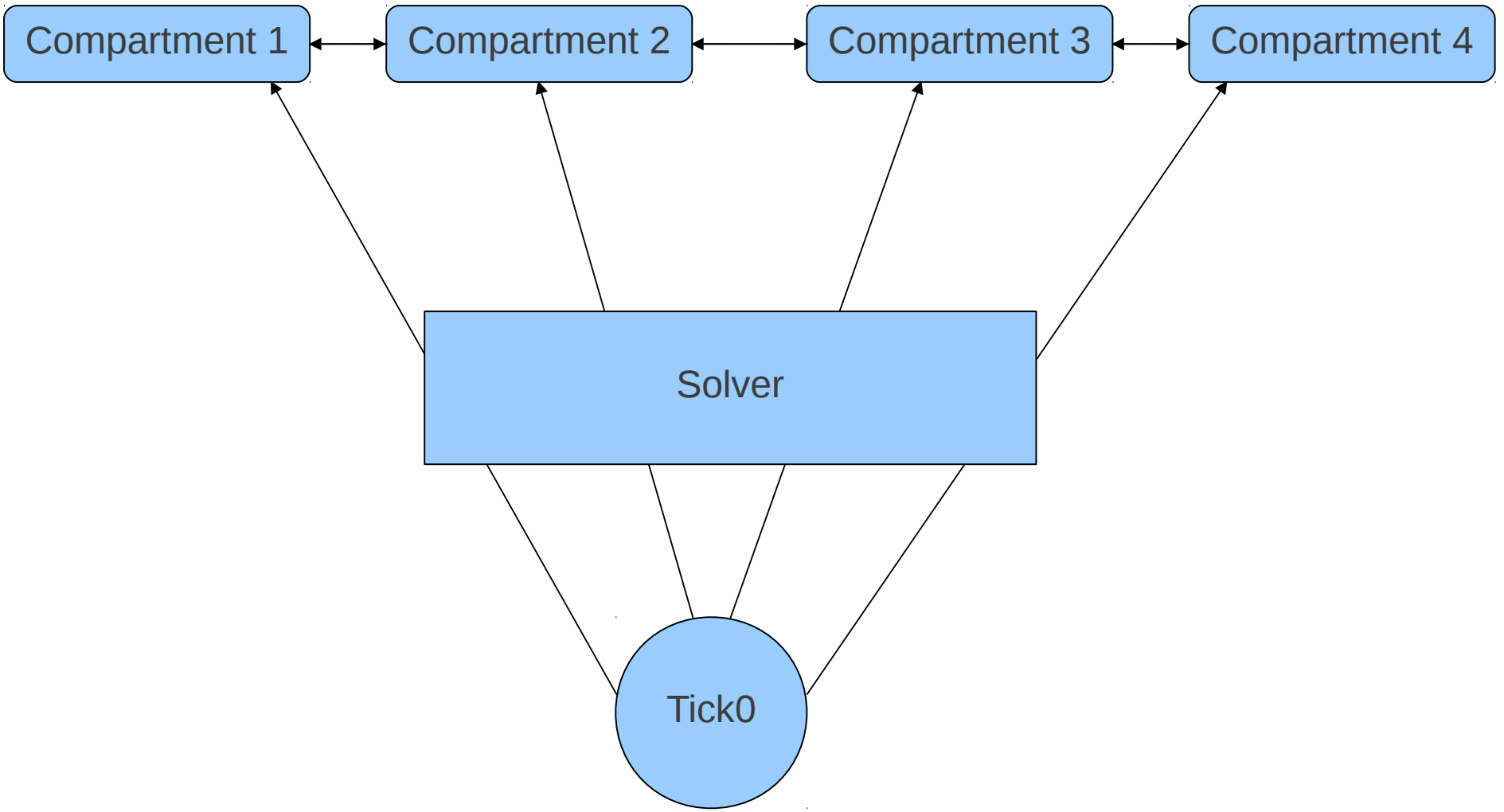

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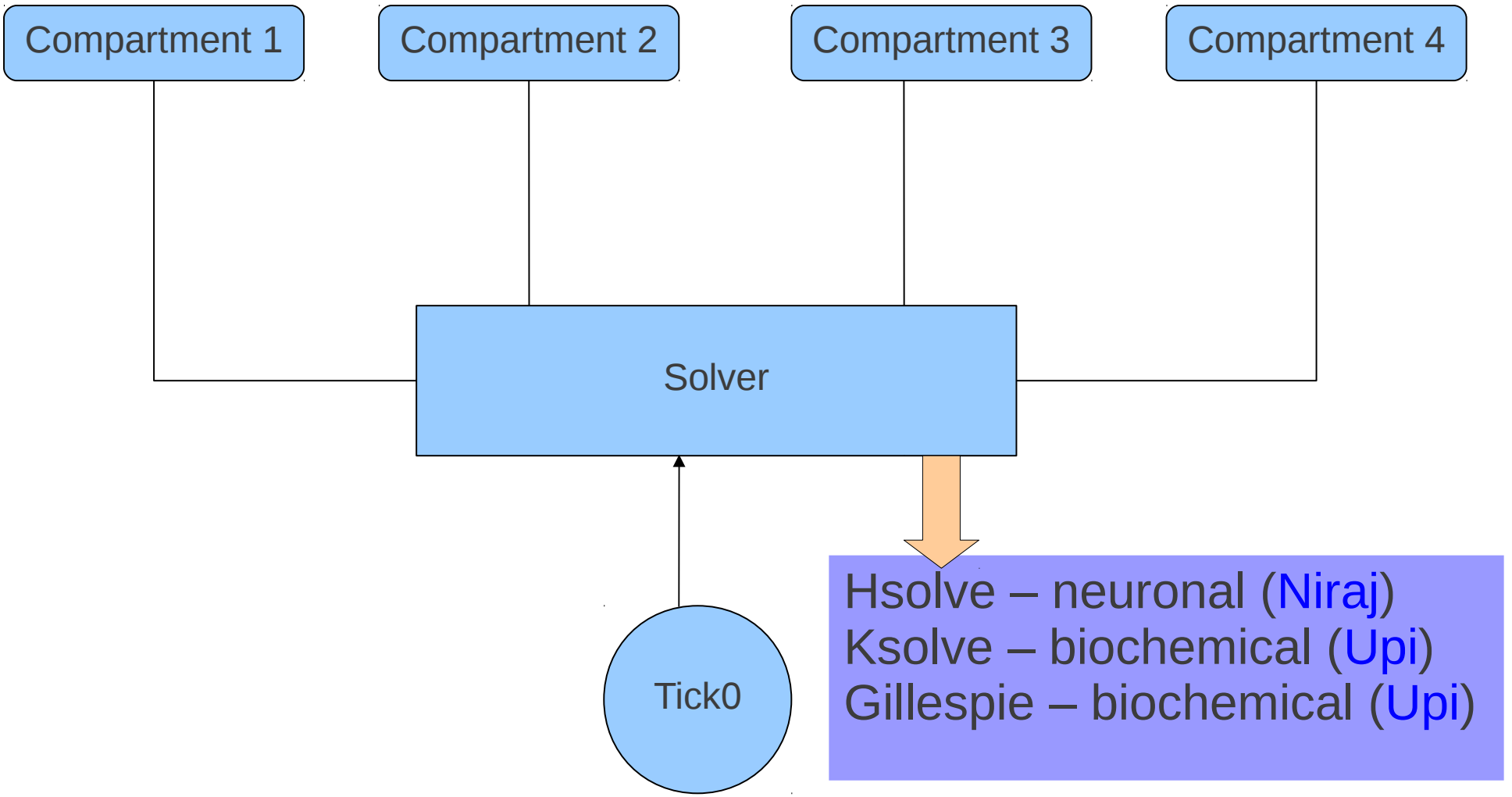

Extensions

- NeuroML and SBML support (9ml partially) (Aditya Gilra, Siji George).
- MUSIC API for *runtime* interaction with other simulators (Niraj Dudani, Johannes Hjorth)
- Smoldyn engine for reaction diffusion systems at cellular scale (Steve Andrews, Upi Bhalla).
- Markov models of ion channels (Vishaka Datta)
- Generally, MOOSE C++ API allows incorporation of other specialized simulation engines as solvers.

New MOOSE: sneak preview

- Complete rewrite applying lessons learned from previous releases.
- Facilities for dynamic class information.
- Focus on utilizing multi-core CPUs and multi-node clusters.

New MOOSE: sneak preview

- Complete switch to Python interface (kinetikit and GENESIS prototype files still supported).
- Computation cleanly separated from user interaction (runs in separate thread). No more blocking during long running simulation.
- Automatic distribution of load among different threads/nodes.
- Most of biophysics and biochemistry classes have been ported. Porting of Hsolve, NeuroML-reader, SBML-reader and the GUI are under development.
- Native support for saving data in HDF5 format.

New MOOSE: sneak preview

- Python interface rewritten using Python/C API
- Much slimmer and more efficient than SWIG-based interface.
- C++ programmer need not worry about Python – it dynamically queries the MOOSE core and generates the class hierarchy using metaprogramming.

Future developments

- Smoldyn support being ported.
- SigNeur – a specialized solver combining signaling models with neuronal models.
- Solvers to utilize GPU for computation in plan.
- Scope for many other solvers at/between various scales.

Join us at:

moose.sourceforge.net
moose.ncbs.res.in

Trying out new moose:

- To check out:

  svn checkout \

  http://moose.svn.sourceforge.net/svnroot/moose/moose/branches/dh_branch/ \

  new_moose
- To compile (needs **g++, make, python-dev, gsl-dev [optional HDF5-dev]**)

  cd new_moose

  make pymoose [optional USE_HDF5=1]
- To try squid axon demo (requires **numpy, PyQt4** and **matplotlib**):

  export PYTHONPATH={path to new_moose}/python:$PYTHONPATH

  cd {path to new_moose}/Demos/squid

  python squid_demo.py

Thank you!

- Upi, Niraj Dudani, Harsharani, Chaitanya, Aditya Gilra and many other contributors to the MOOSE project.
- NCBS/TIFR, DAE/SRC, INCF, SBCNY