Reproducible Models and Replicable Implementations

Current Trends in Computational Neuroscience

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Presented at SIAM Computational Science & Engineering
Reno, NV, 4 March 2011

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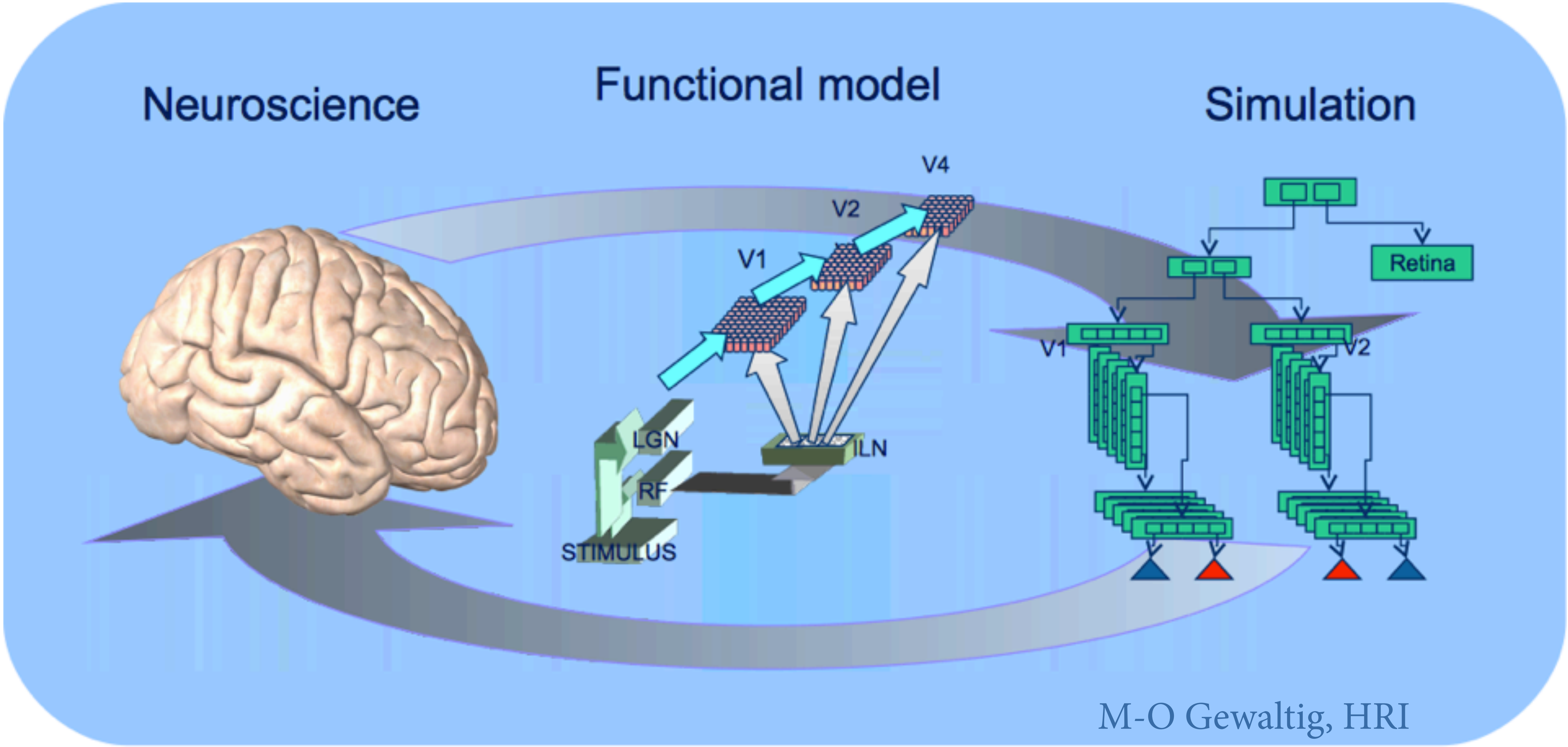
MDCCCLIX

Computational Neuroscience

What is Computational Neuroscience?



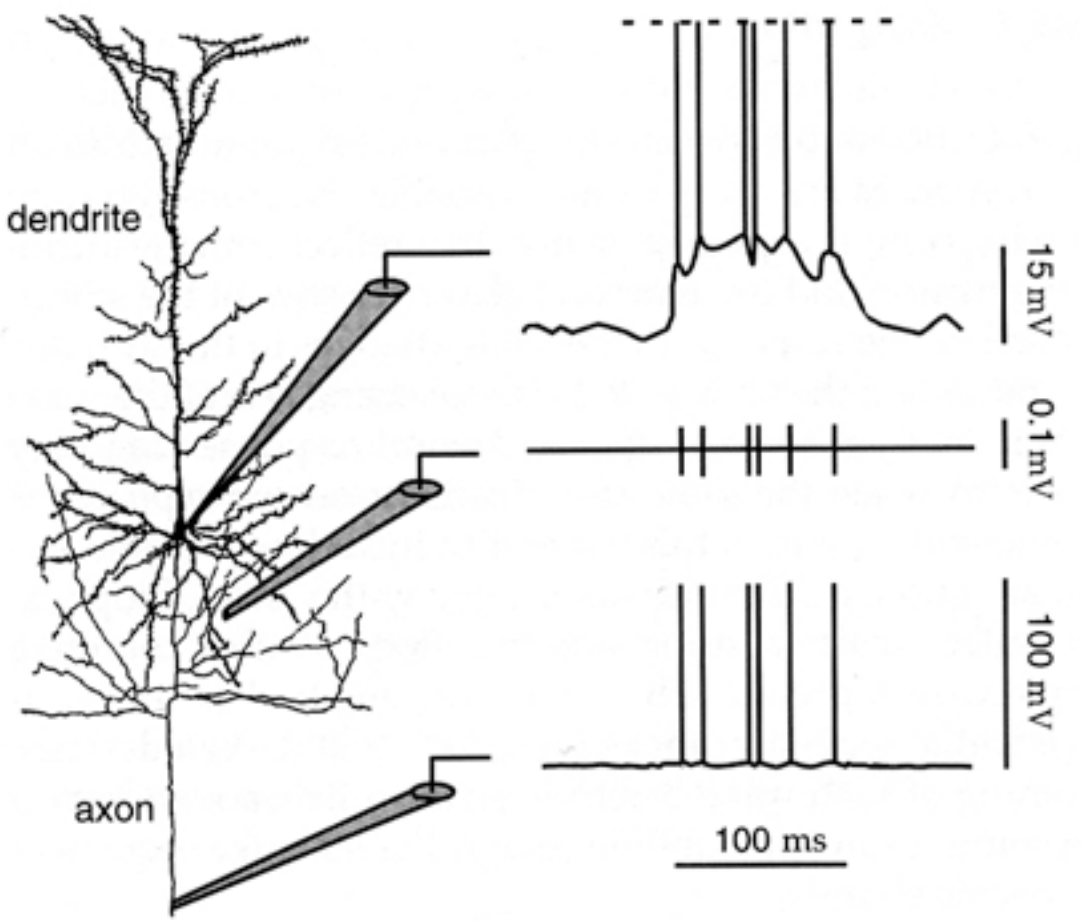
M-O Gewaltig, HRI

The goal of neural modeling is to relate, in nervous systems, function to structure on the basis of operation.

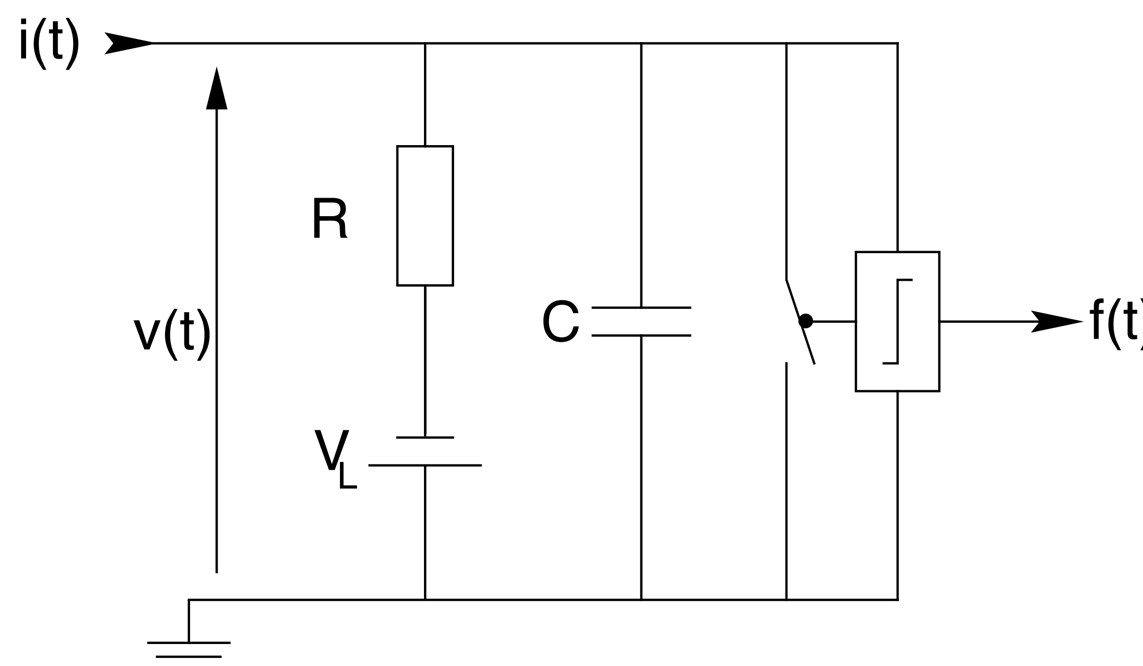
MacGregor & Lewis, 1977

Keeping it simple: point neurons

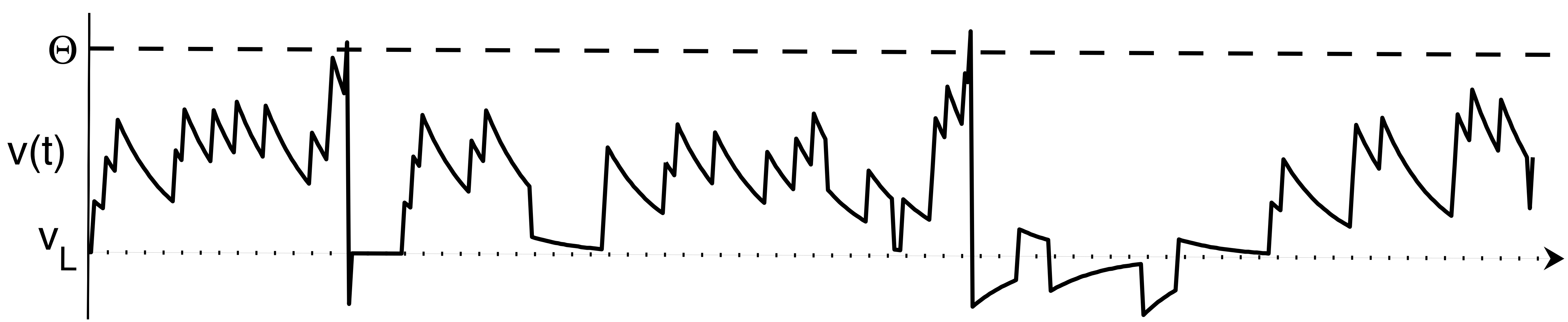
Complexity of the neuron



… abstracted as simple RC-circuit

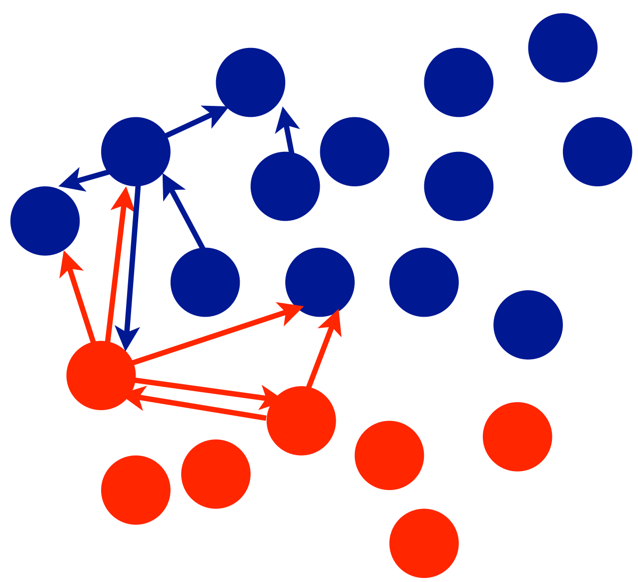


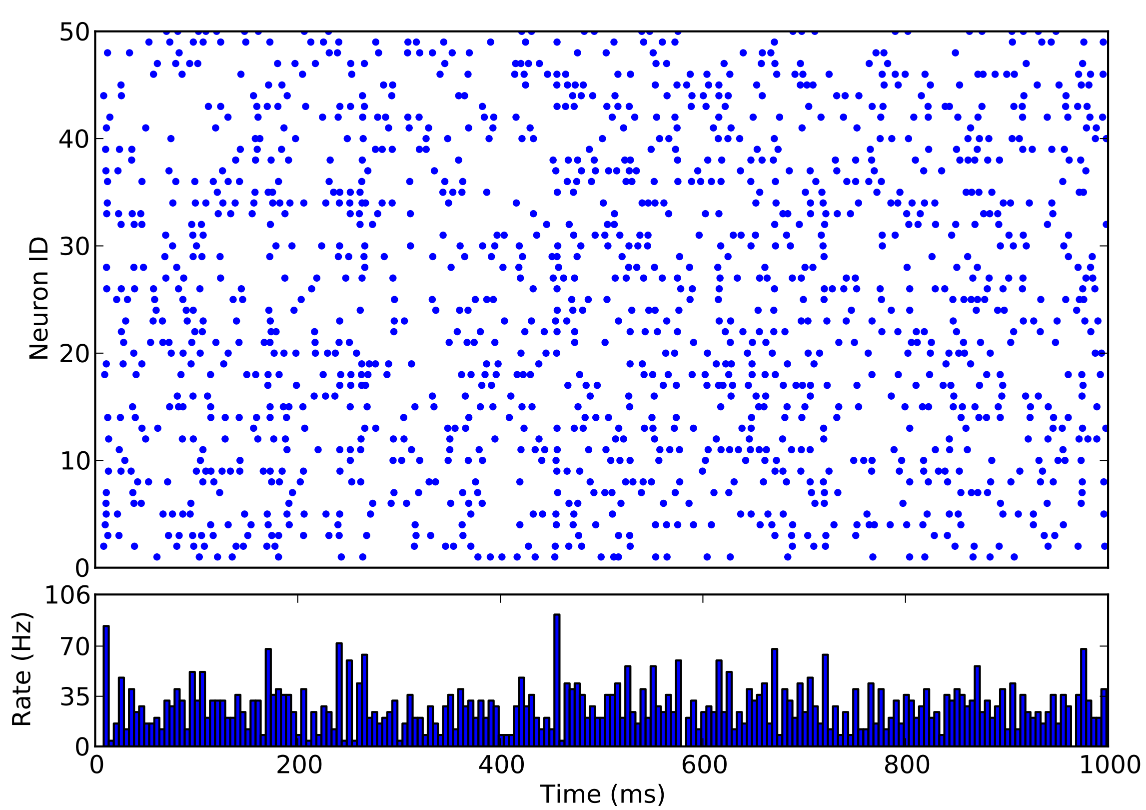
$$C\dot{V} = -\frac{(V - V_L)}{R} + i(t)$$



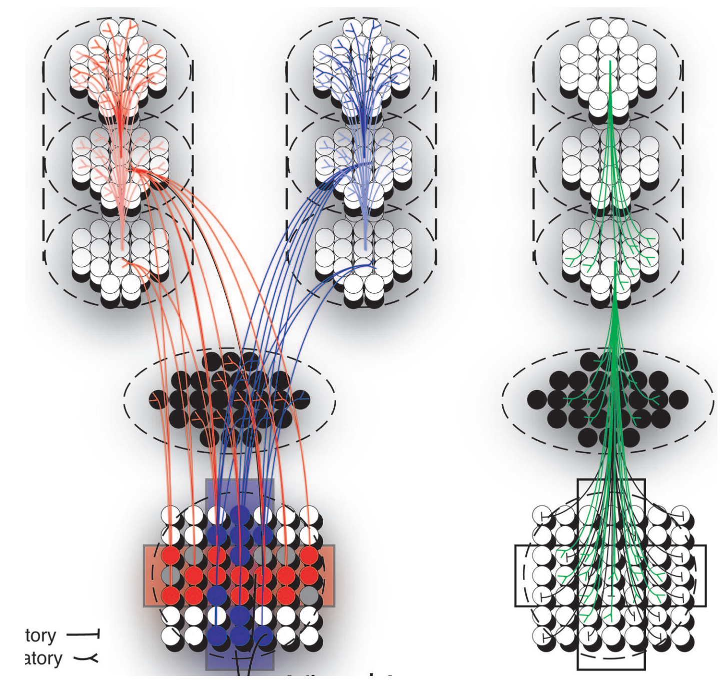
Then explore network dynamics!

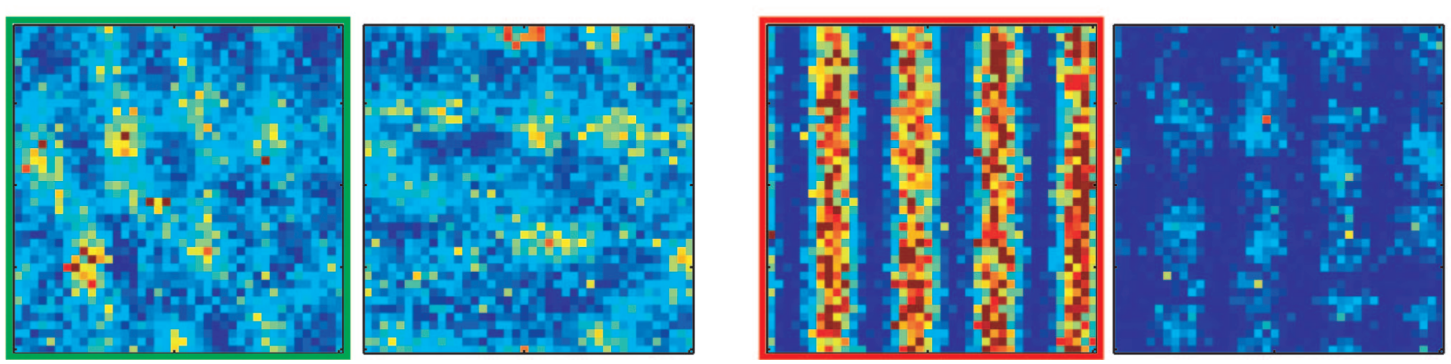
Random network





Structured network





Hill & Tononi (2005)

Simulations are exciting — but reliable?

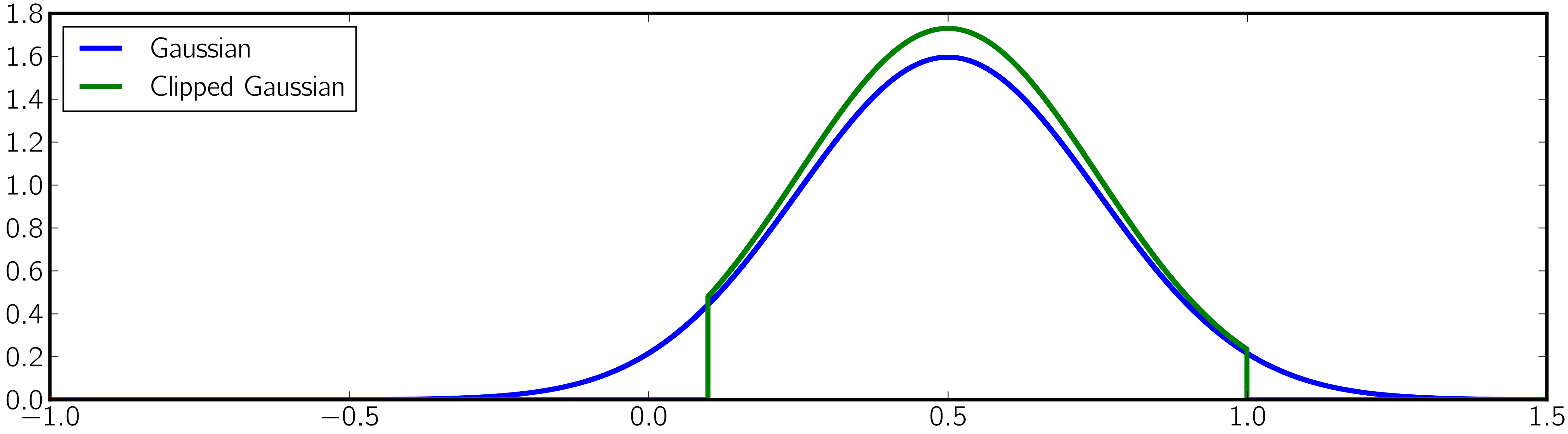
- Computational neuroscience
  - no conservation laws
  - no clear-cut separation of scales
  - no general agreement on which aspects of network activity are essential (spike rate vs spike time debate)
  - highly abstract models difficult to compare to experimental data quantitatively

➡Highly dependent on *reliable* simulations

➡Let's look at a real-life case

Case 2: The clipped Gaussian

- Well-known paper on plasticity
- Parameters chosen from Gaussian distribution, according to paper
- Results could not be reproduced independently
- Analysis of original C-code provided by authors:
  - ➡Parameters were chosen from *clipped* Gaussian



The (sad) state of the art

- Few published results can be reproduced independently
- Authors often struggle to replicate their own results
- Systematic comparison and evaluation of models are rare
- Authors rarely discuss why and how models ended up as they are
- Models are seldom re-used

Reproduction *vs* Replication

Chris Drummond

Replicability is not Reproducibility: Nor is it Good Science

ICML Montreal 2009

Replication: necessary, difficult, & insufficient

- Replication
  - Re-create identical results
  - Essentially book-keeping
  - Requires tools & discipline
  - No new insights: tests implementation, not ideas
- *Internal replication*
  Joe recreates results on original machine
- *External replication*
  Jane recreates Joe's results on her machine using Joe's code
- *Cross replication*
  Alice recreates Joe's results using a different simulator, based on a simulator-independent model description

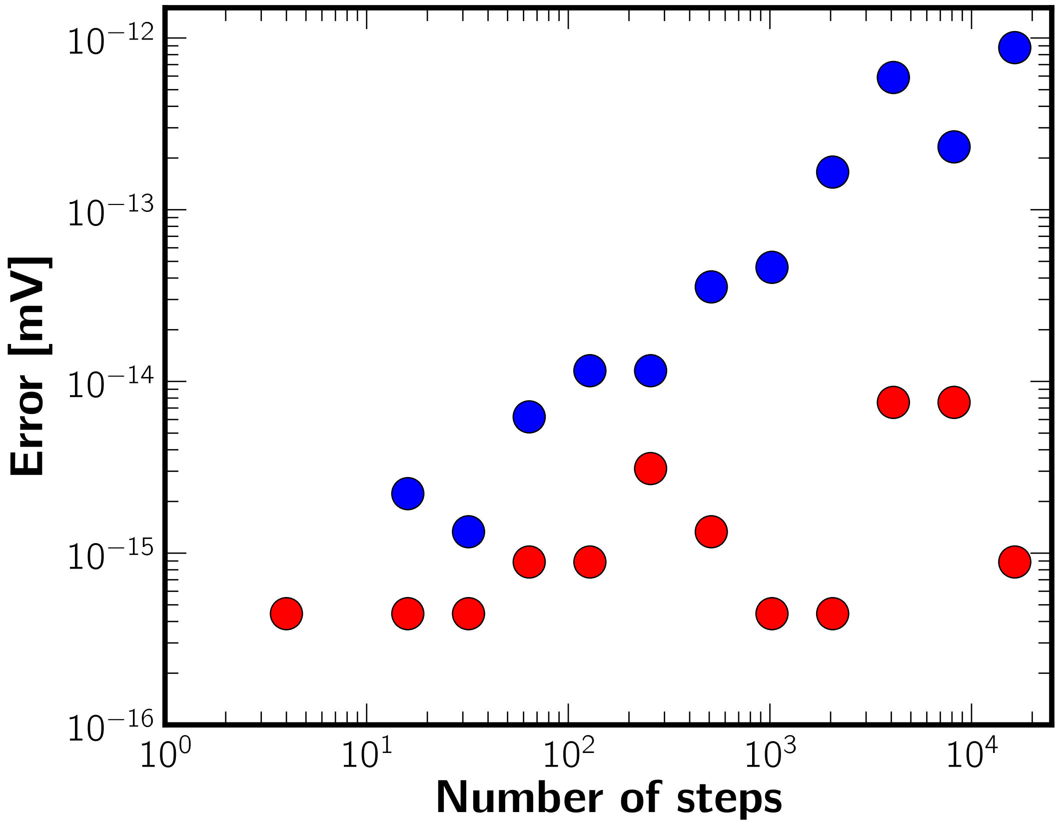
How much detail does replication require?

- Very simple point-neuron model

$$\dot{V} = -\frac{V}{\tau} + \frac{I_E}{C}$$

- Exact updating rule ($a = I_E \tau / C$)

$$V_{k+1} = V_k e^{-h/\tau} + a(1 - e^{-h/\tau})$$



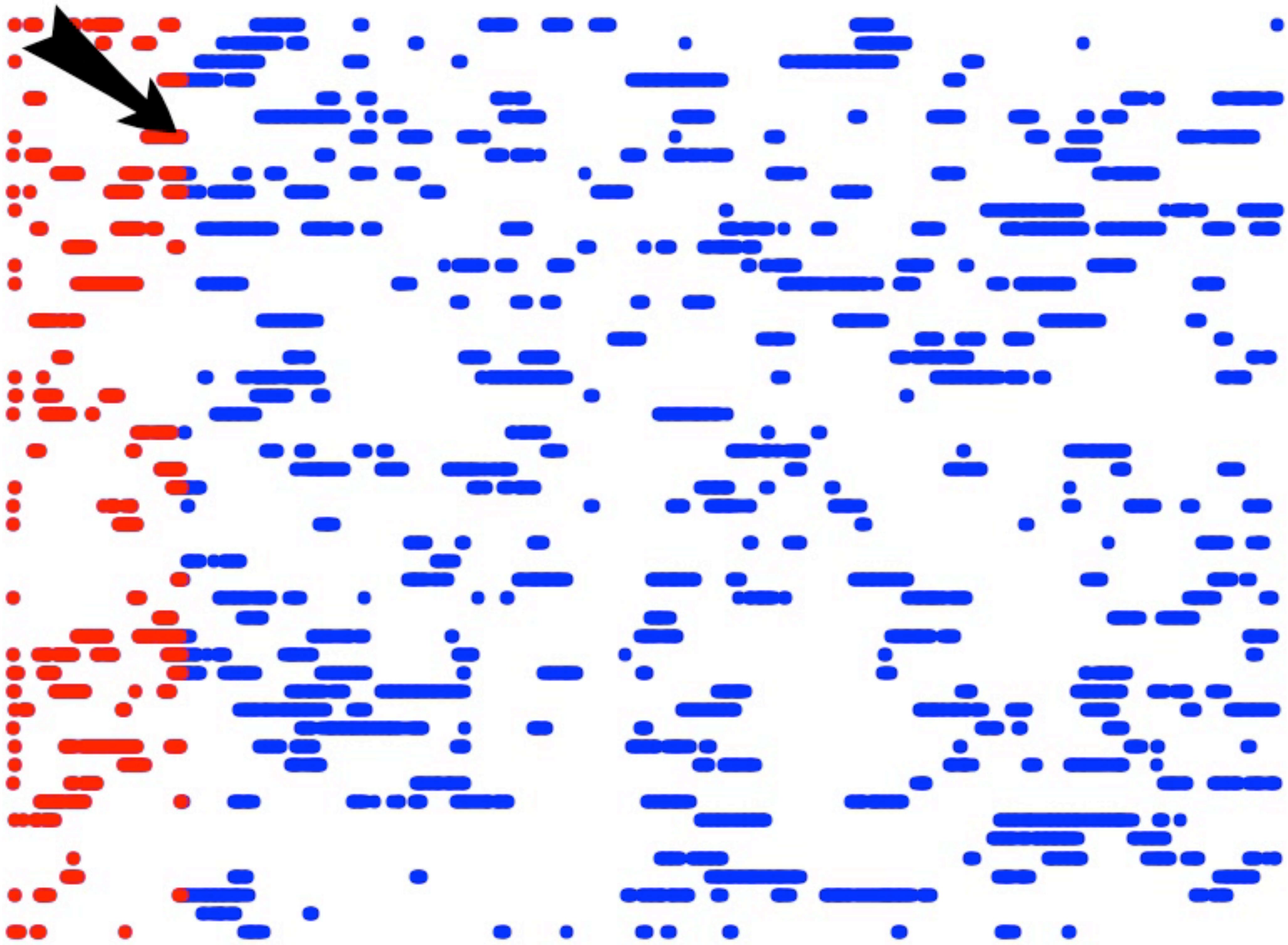
- Two different implementations

```
V[k+1] = V[k] * exp(-h/tau) - a * expm1(-h/tau)
V[k+1] = V[k] - (a - V[k]) * expm1(-h/tau)
```

- Different numerical properties

➡ Replication requires that we specify implementation!

But do such tiny differences matter?

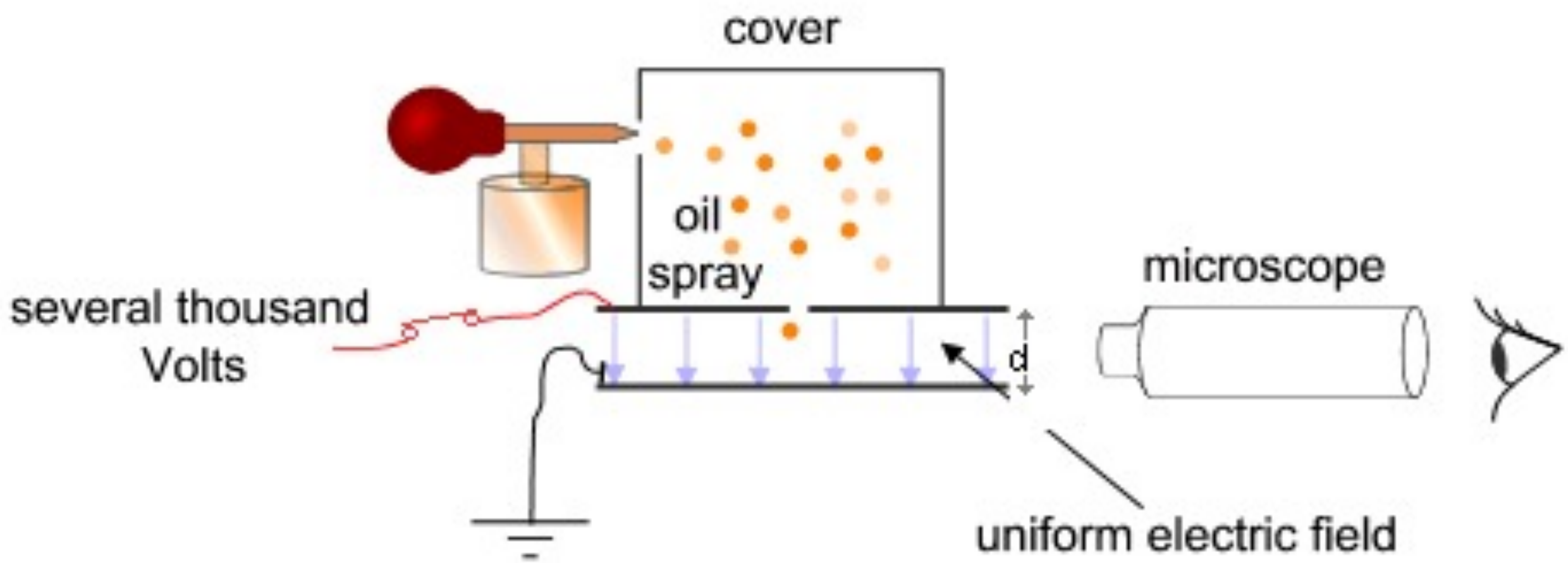


Reproduction

- Independent
- Test hypotheses and models
- Validates concepts
- Requires reflection

From oil drops to first-passage times

Millikan's oil drop experiment



Wikipedia

Erwin Schrödinger
Zur Theorie der Fall- und Steigversuche an Teilchen mit Brownscher Bewegung
Physikalische Zeitschrift **16**:289 (1915)

Reproduction needs replication

- Reproducible models describe scientific ideas
- Independent reproduction will generally fail to replicate original results precisely
- Requires learned judgement of discrepancies
- Requires means to understand failure

➡ Replicable implementation

Improving Scientific Practice in Computational Neuroscience

Good model description practice

- Systematic approach to model description in papers
- Standardize tables/checklists
- Standards for graphic representation of models
- Nordlie, Gewaltig, & Plesser *PLoS Comp Biol* **5**:e1000456 (2009)

A	Model Summary
Populations	Three: excitatory, inhibitory, external input
Topology	—
Connectivity	Random convergent connections
Neuron model	Leaky integrate-and-fire, fixed voltage threshold, fixed absolute refractory time (voltage clamp)
Channel models	—
Synapse model	α-shaped current inputs
Plasticity	—
Input	Independent fixed-rate Poisson spike trains to all neurons (during initial stimulation period)
Measurements	Spike activity

B	Populations	
Name	**Elements**	**Size**
E	Iaf neuron	$N_E = 4N_I$
I	Iaf neuron	N_I
E_{ext}	Poisson generator	$C_E(N_E + N_I)$

C	Connectivity		
Name	**Source**	**Target**	**Pattern**
EE	E	E	Random convergent $C_E \to 1$, weight J, delay D
IE	E	I	Random convergent $C_E \to 1$, weight J, delay D
EI	I	E	Random convergent $C_I \to 1$, weight $-gJ$, delay D
II	I	I	Random convergent $C_I \to 1$, weight $-gJ$, delay D
Ext	E_{ext}	$E \cup I$	Non-overlapping $C_E \to 1$, weight J, delay D

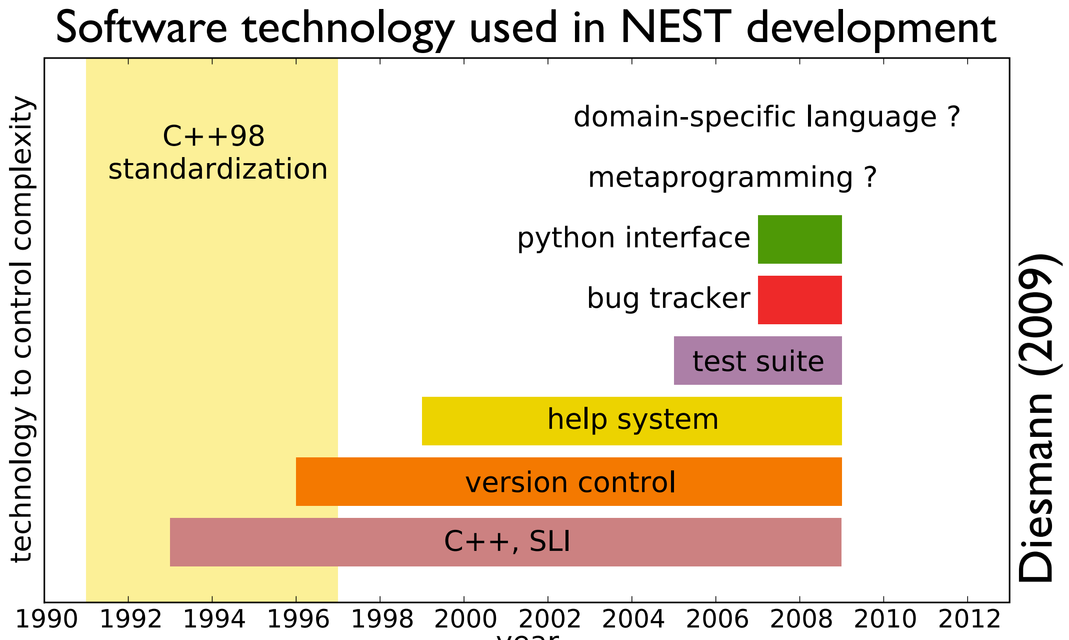
D	Neuron and Synapse Model
Name	Iaf neuron
Type	Leaky integrate-and-fire, α-current input
Subthreshold dynamics	$\tau\dot{V}(t) = -V(t) + RI(t)$ if $t > t^* + \tau_{rp}$; $V(t) = V_r$ else; $I(t) = \frac{\tau}{R}\sum_{\tilde{t}} w\alpha(t - (\tilde{t} + \Delta))\Theta(t - (\tilde{t} + \Delta))$
Spiking	If $V(t-) < \theta \wedge V(t+) \geq \theta$ 1. set $t^* = t$ 2. emit spike with time-stamp t^*

E	Input
Type	**Description**
Poisson generators	Fixed rate ν_{ext}, C_E generators per neuron, each generator projects to one neuron; active only during initial stimulation period

F	Measurements
Spike activity as raster plots for subset of excitatory neurons

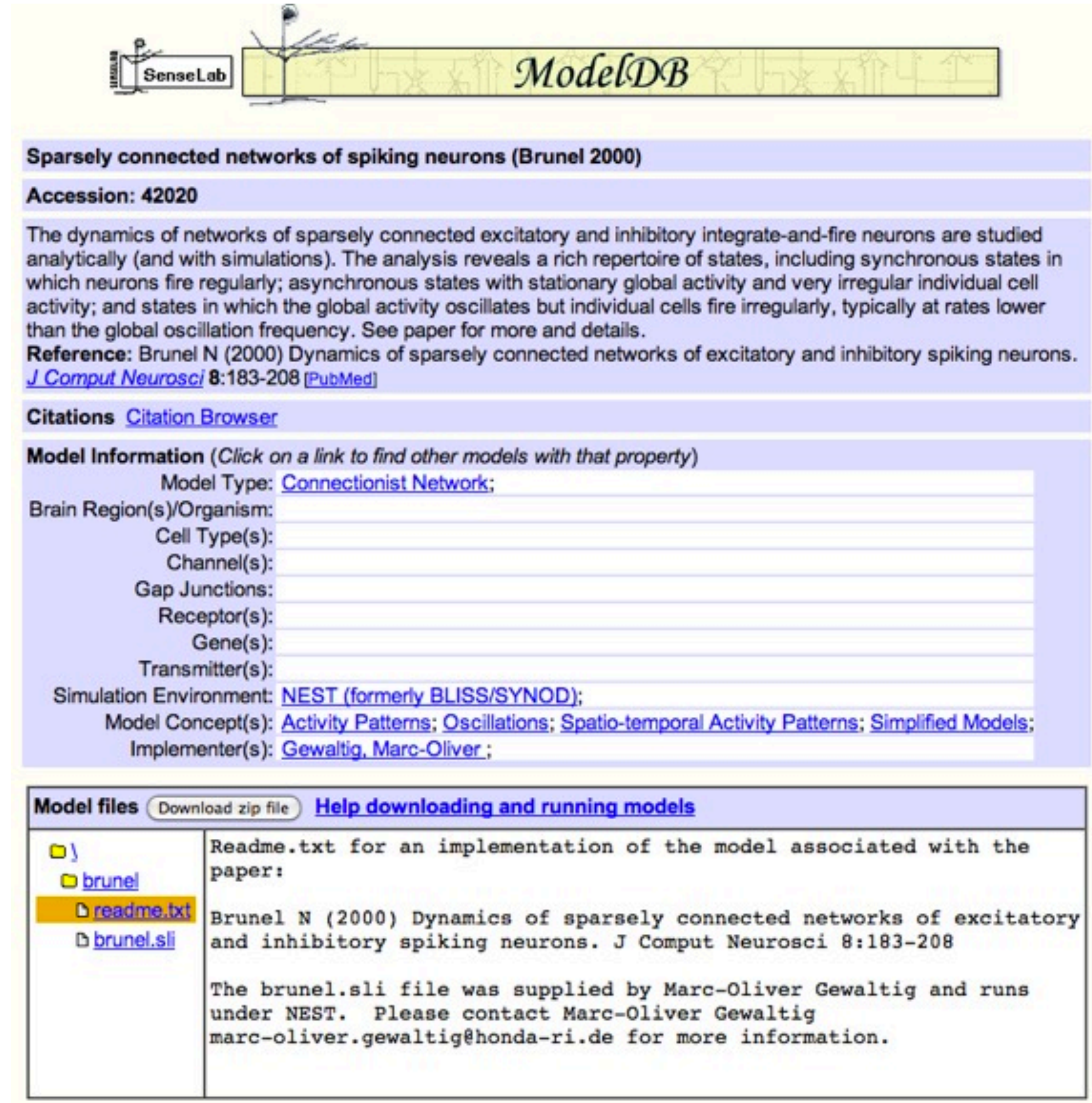
Professional, shared software

- Widely used packages replace homemade *ad hoc* code
- Currently: Neuron, NEST, Genesis, Moose, Brian, PCSim
- "Social" developments
  - Simulator review (Brette *et al*, 2007)
  - Teaching software at summer schools
  - Large-scale *scientific* projects (eg EU FACETS)
  - Neuroinformatics journals
  - Raising awareness among reviewers and editors
- "Technical" developments
  - Version control
  - Test suites



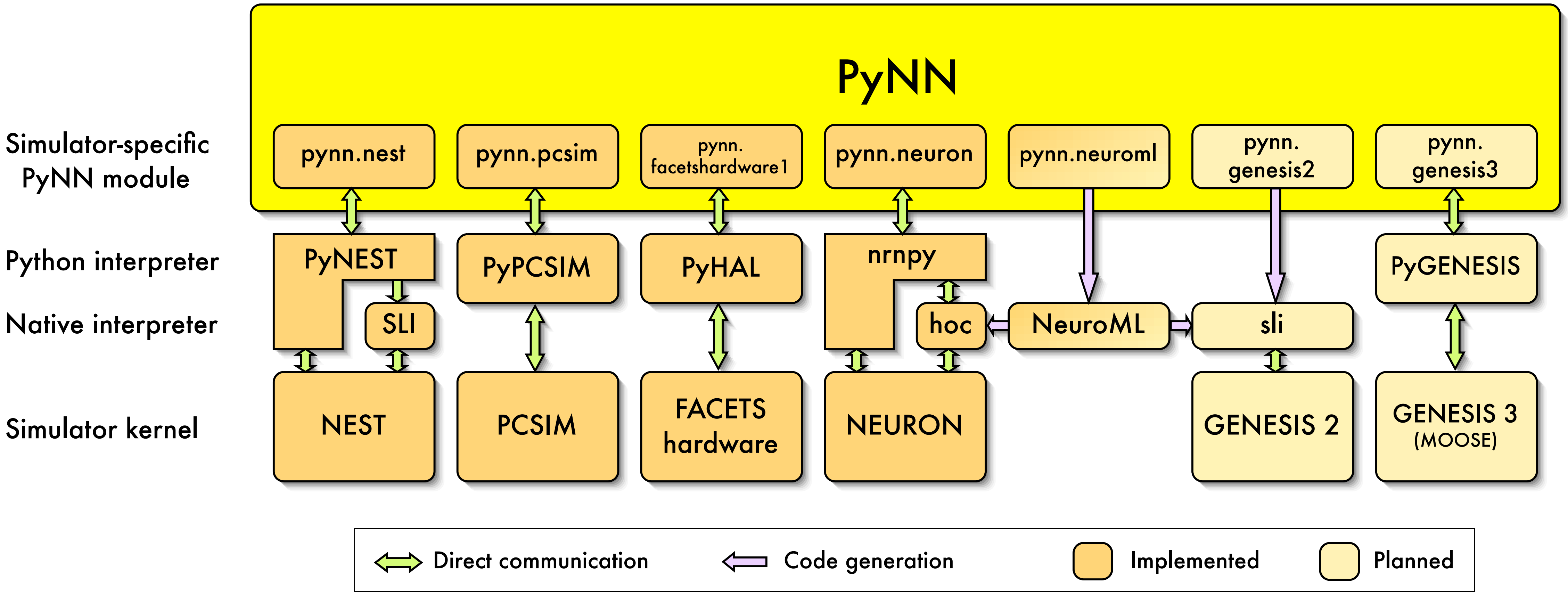
ModelDB: Sharing models

- Curated database of computational neuroscience models
- Only published models
- Open to any software
- Nearly 700 models
- http://senselab.med.yale.edu/modeldb/



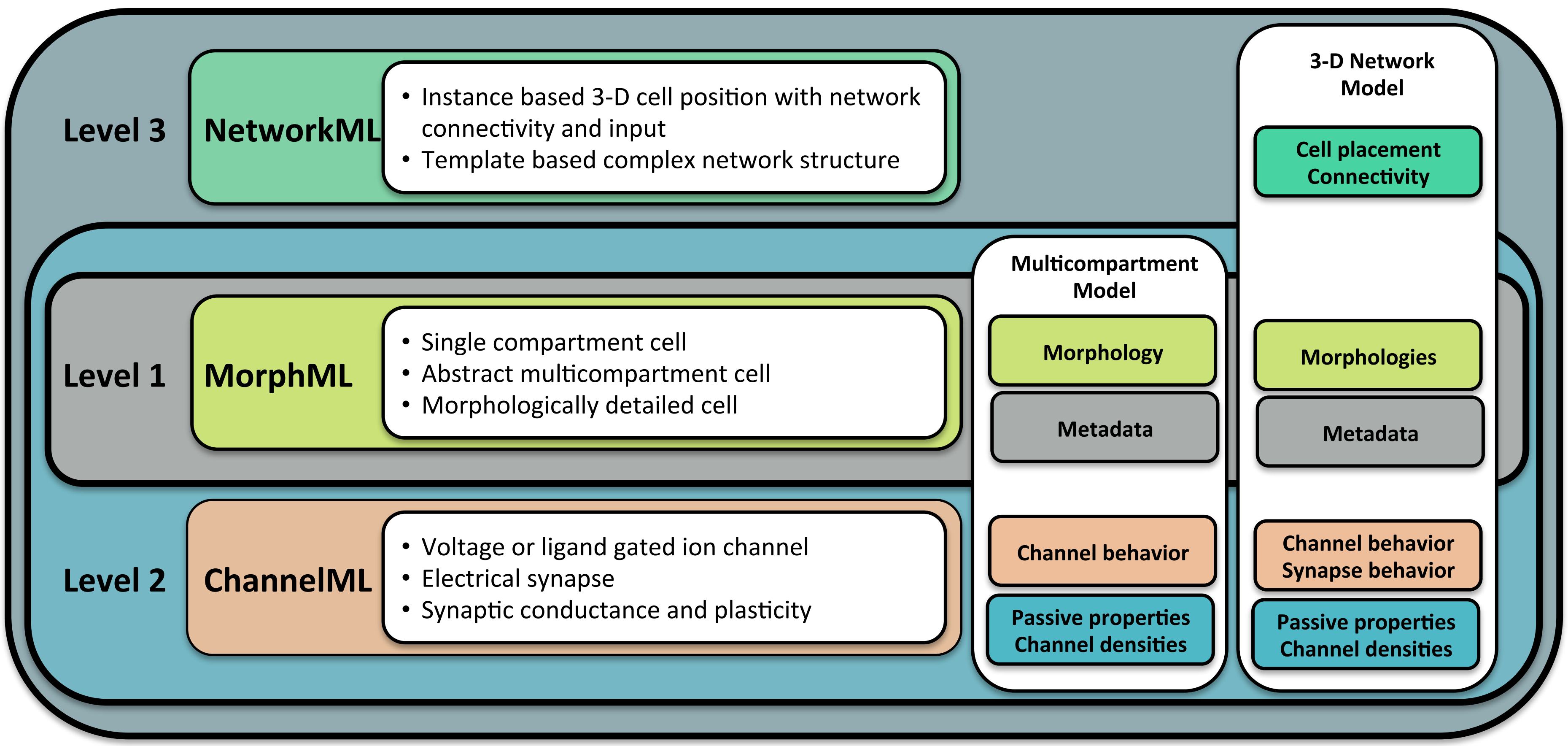
PyNN: A Meta-Simulator

- Python-based wrapper for many simulators
- Write model and simulation code once, run on all
- Facilitates model sharing and cross-validation
- Developed by Andrew Davison for FACETS project
- http://neuralensemble.org/PyNN



NeuroML: A model specification language

- XML-based language for model specification
- Multiple layers: channels, neuron morphologies, networks
- Code-generation for several simulators, including PyNN
- Facilitates model sharing and re-use
- http://www.neuroml.org



Provenance tracking: Sumatra

- Python package to enable systematic capture of the environment of numerical simulations/analyses
- Tracks simulation code, dependencies, platform information, results
- Developed by Andrew Davison as part of FACETS project
- http://neuralensemble.org/sumatra

Sumatra: TestProject: List of records

http://127.0.0.1:8002/

TestProject: List of records

Delete include data	Label	Reason	Outcome	Duration	Processes	Simulator		Script			Date	Time	Tags
						Name	Version	Repository	Main file	Version			
☐	20100709-154255		'Eureka! Nobel prize here we come.'	0.59 s		Python	2.5.2	/Users/andrew/tmp/SumatraTest	main.py	396c2020ca50	09/07/2010	15:42:55	
☐	20100709-154309			0.59 s		Python	2.5.2	/Users/andrew/tmp/SumatraTest	main.py	396c2020ca50	09/07/2010	15:43:09	
☐	haggling	'determine whether the gourd is worth 3 or 4 shekels'	'apparently, it is worth NaN shekels.'	0.59 s		Python	2.5.2	/Users/andrew/tmp/SumatraTest	main.py	396c2020ca50	09/07/2010	15:43:20	foobar

NineML: A model description standard

- Aims for community standard for declarative model descriptions
- Inspired by SBML and CellML
- Focus on networks of point neurons
- Under development by INCF Multi-scale Modeling Task Force

Perspectives

- Community increasingly aware of need for reproducibility and replicability
- Large-scale projects have led to development of valuable tools
- Summer schools educate PhD-students and post-docs in use of established modeling tools
- Neuroinformatics journals allow publication of domain-specific solutions
- International Neuroinformatics Coordinating Facility (INCF) stimulates debate and development
- NEST Initiative is devoted to furthering reliable simulations

➡ We have a long way to go, but we are (finally) moving!

Collaborators

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Marc-Oliver Gewaltig

Honda Research Institute Europe
Offenbach

nest:: initiative

Research Council of Norway (eVita program)