nest::

THE NEURAL SIMULATION TOOL NEST

1st HPAC Platform Training

December 11, 2018 | Jochen M. Eppler (j.eppler@fz-juelich.de) | SimLab Neuroscience

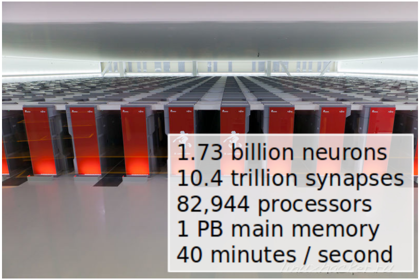
OUTLINE

- Introduction
- Neuronal simulations
- Technological background
- Developing new models
- Performance

NEST = NEURAL SIMULATION TOOL

- Point neurons and neurons with few electrical compartments
- Phenomenological synapse models (STDP, STP)
  - + gap junctions, neuromodulation and structural plasticity
- Frameworks for rate models and binary neurons
- Support for neuroscience interfaces (MUSIC, libneurosim)

- Highly efficient C++ core with a Python frontend
- Hybrid parallelization (OpenMP+MPI)
- Same code from laptops to supercomputers



1.73 billion neurons
10.4 trillion synapses
82,944 processors
1 PB main memory
40 minutes / second

NEST DESIGN GOALS

High accuracy and flexibility

- Each neuron model is assigned an appropriate solver
- Exact integration is used for suitable neuron models
- Spikes are usually restricted to the computation time grid
- Spike interaction in continuous time for some models

Constant quality assurance

- Automated unittest suite included in NEST build
- Continuous integration for all repository checkins
- Code review for all code contributions

NEST's development is always driven by scientific needs

WHEN TO USE NEST?

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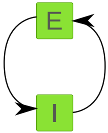
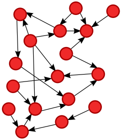
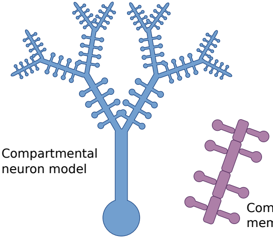
Population model



Point neuron network model

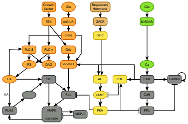


Compartmental neuron model



Compartmental membrane model

Reaction-diffusion model



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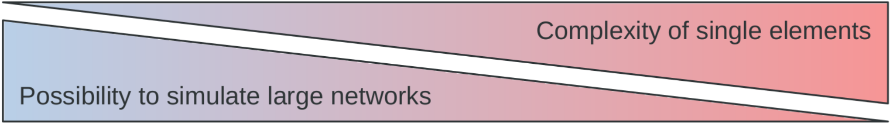
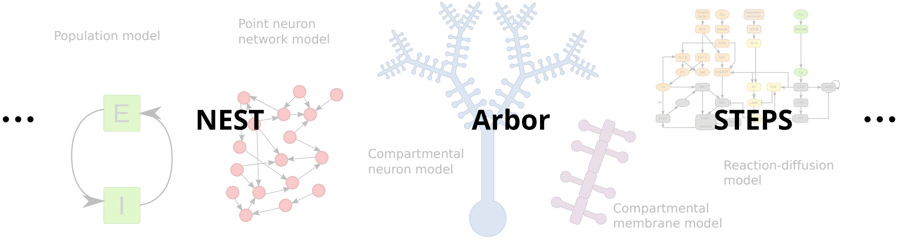
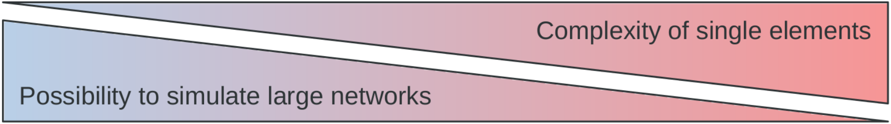


WHEN TO USE NEST?





Complexity of single elements

Possibility to simulate large networks

OBTAINING NEST

Download from `http://nest-simulator.org`

- Source code for official releases
- Virtual machine images (e.g. for use on Windows)

Open source development:

- `https://github.com/nest/nest-simulator`
- Direct access to current and future development
- Ability to fork and develop locally
- Pull requests for merging into the official version

From your distribution’s package repository:

- PPA for Ubuntu and Debian
- Package in Neuro-Fedora

INSTALLING FROM SOURCE (LINUX)

1. **Download NEST and unpack** (in `$HOME` folder)**:**

```
wget https://git.io/vFxDo
tar -xzvf nest-2.14.0.tar.gz
```

2. **Create and enter build directory:**

```
mkdir nest-2.14.0-bld
cd nest-2.14.0-bld
```

3. **Configure, compile and install build:**

```
cmake -DCMAKE_INSTALL_PREFIX=$HOME/nest-2.10.0-inst ../nest-2.14.0
make -j4
make install
```

4. **Update environment** (in `$HOME/.bashrc` or similar file)**:**

```
. $HOME/nest-2.14.0-inst/bin/nest_vars.sh
```

NEST LIVE MEDIA USING VIRTUALBOX

1. **Download and install VirtualBox:** `http://virtualbox.org`
2. **Download NEST live media:** `http://nest-simulator.org/download`
    - Includes NEST, NEURON, Brian, PyNN, ...
3. **Start VirtualBox**:
    - File → Import Appliance → Appliance to import → Open
4. **Start VM, install VirtualBox Guest Additions CD image** (Devices →). Follow instructions and restart guest OS
5. **Set up shared folders** (between host and guest):
    - Create shared folder in host OS, e.g. `vb_shared`
    - Devices → Shared Folders → Settings: add new
    - Uncheck 'Auto-mount' and 'Make permanent' → OK → OK
    - Create mount point in guest OS:

```
mkdir sharedir
sudo mount t vboxsf o uid=999,gid=999 vb_shared sharedir
```

HELP!

Within Python:

```
nest.help()
nest.helpdesk()
nest.help('iaf_psc_exp')
nest.help('Connect')
```

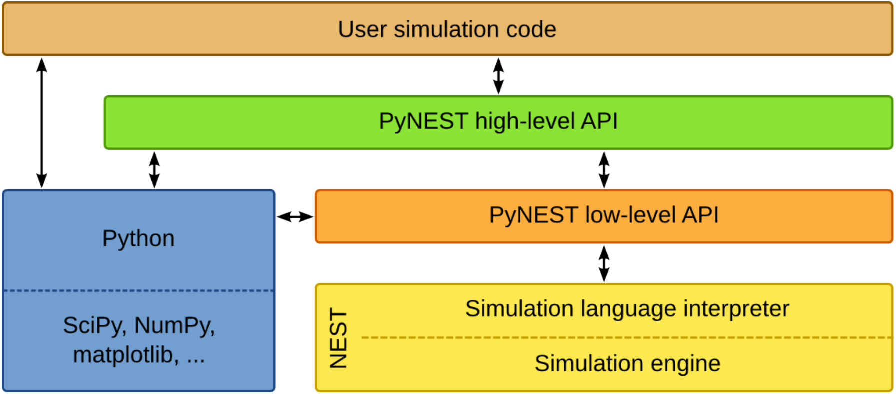
Online documentation:

`http://nest-simulator.org/documentation`

Community:

- NEST user mailing list
- Bi-weekly open video conference
- `http://nest-initiative.org/community`

HOW TO USE NEST?



User simulation code

PyNEST high-level API

Python

SciPy, NumPy, matplotlib, ...

PyNEST low-level API

NEST

Simulation language interpreter

Simulation engine

Different user interfaces for maximum flexibility

HOW TO USE NEST?

Two different command line user interfaces:

- The built-in simulation language interpreter SLI

```
/n iaf_psc_alpha << /V_m -50.0 >> 5 Create def
/sd spike_detector Create def
n sd Connect
```

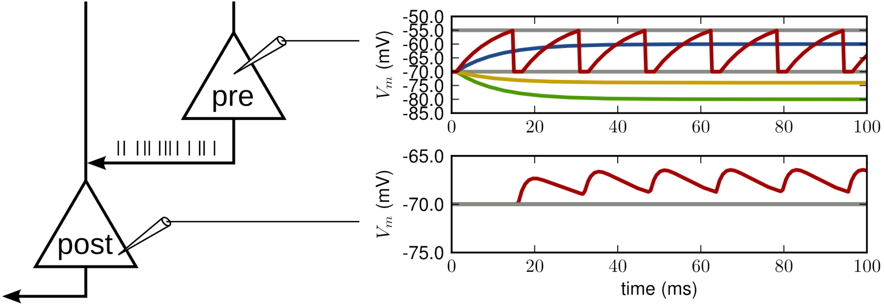
- The Python interface PyNEST

```
n = nest.Create("iaf_psc_alpha", 5, {"V_m": -50.0})
sd = nest.Create("spike_detector")
nest.Connect(n, sd)
```

NEST is also supported by the multi-simulator interface PyNN

NEURONAL SIMULATIONS IN NEST

A simulation in NEST mimics a neuroscientific experiment



NEURONAL SIMULATIONS IN NEST

- The network in NEST comprises a directed, weighted graph
  - Nodes represent either neurons or devices
  - Edges represent synapses between nodes
- Nodes are updated on a fixed-time grid, while spikes can also be in continuous time
- Neurons can be arbitrarily complex, not just point neurons
- Devices for stimulating neurons and recording their activity
- Synapse models to establish connections between nodes
- Parallelization and inter-process communication is handled transparently by NEST

NEURON MODELS

- Integrate-and-fire models (`iaf_`)
    - Current-based (`iaf_psc`)
    - Conductance-based (`iaf_cond`)
    - Different post-synaptic shapes (`_alpha`, `_exp`, `_delta`)
- Single compartment Hodgin-Huxley models (`hh_`)
- Adaptive exponential integrate-and-fire models (`aeif_`)
- MAT2 neuron model (Kobayashi et al. 2009)
- Neuron models with few compartments

- Creation of neurons using the `Create` command:

```
Create(<model>, <num>, <params>)
```

STIMULATION DEVICES

Spike generators:

- `spike_generator` spikes at prescibed points in time
- `poisson_generator` spikes according to a Poisson distribution
- `gamma_sup_generator` spikes according to a Gamma distribution

Current generators

- `ac_generator` provides a sine-shaped current
- `dc_generator` provices a constant current
- `step_current_generator` provides a step-wise constant current
- `noise_generator` provides a random noise current

RECORDING DEVICES

- `spike_detector` records incoming spikes
- `multimeter` records analog quantities (potentials, conductances, ...)
- `voltmeter` records the membrane potential
- `correlation_detector` records pairwise cross-correlations between the spiking activity of neurons
- `weight_recorder` records the weight of connections

GENERAL PARAMETER ACCESS

All parameter access in NEST is carried out via dictionaries

- Retrieving the status of an element:

```
GetStatus(<element(s)>)
GetStatus(<element(s)>, <key(s)>)
```

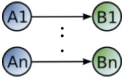
- Setting properties of an element:

```
SetStatus(<element(s)>, <dict(s)>)
SetStatus(<element(s)>, <key(s)>, <value(s)>)
```

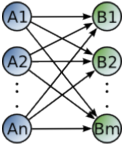
SPECIFICATION OF CONNECTIVITY

The Parameter conn_spec:

- defines the connection rule
- defines rule-specific parameter
- can be a string or a dictionary



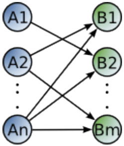
```
A = Create('iaf_psc_alpha', n)
B = Create('spike_detector', n)
Connect(A, B, 'one_to_one')
```



```
A = Create('iaf_psc_alpha', n)
B = Create('iaf_psc_alpha', m)
Connect(A, B)
```

SPECIFICATION CONNECTIVITY

```
A = Create("iaf_psc_alpha", n)
B = Create("iaf_psc_alpha", m)
conn_dict = {'rule': 'fixed_indegree',
             'indegree': N}
Connect(A, B, conn_dict)
```



Further rules and their keys:

- ’fixed_outdegree’, ’outdegree’
- ’fixed_total_number’, ’N’
- ’pairwise_bernoulli’, ’p’

SPECIFICATION OF SYNAPSE PROPERTIES

Using customized synapse model:

```
A = Create('iaf_psc_alpha', n)
B = Create('iaf_psc_alpha', n)
CopyModel('static_synapse','excitatory',
           {'weight':2.5, 'delay':0.5})
Connect(A, B, syn_spec='excitatory')
```

Insert synapse parameter directly into Connect():

```
syn_dict = {'model': 'static_synapse',
            'weight': 2.5, 'delay': 0.5}
Connect(A, B, syn_spec=syn_dict)
```

syn_spec defines the synapse model and synapse-specific parameters and can be a string or a dictionary

RANDOMIZATION OF SYNAPSE PROPERTIES

- specify distributed parameters as dictionaries

```
delay_dist = {'distribution': 'uniform',
              'low': 0.8, 'high': 2.5}

alpha_dist = {'distribution': 'normal_clipped',
              'low': 0.5, 'mu': 5.0,
              'sigma': 1.0}

syn_dict = {'model': 'stdp_synapse',
            'weight': 2.5,
            'delay': delay_dist,
            'alpha': alpha_dist}
```

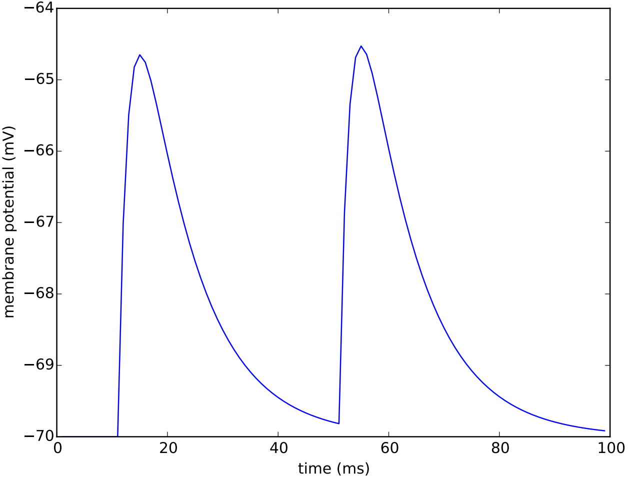
DISTRIBUTIONS

Distributions	Keys
’normal’	’mu’, ’sigma’
’normal_clipped’	’mu’, ’sigma’, ’low ’, ’high’
’lognormal’	’mu’, ’sigma’
’lognormal_clipped’	’mu’, ’sigma’, ’low’, ’high’
’uniform’	’low’, ’high’
’uniform_int’	’low’, ’high’
’binomial’	’n’, ’p’
’binomial_clipped’	’n’, ’p’, ’low’, ’high’
’exponential’	’lambda’
’exponential_clipped’	’lambda’, ’low’, ’high’
’gamma’	’order’, ’scale’
’gamma_clipped’	’order’, ’scale’, ’low’, ’high’
’poisson’	’lambda’
’poisson_clipped’	’lambda’, ’low’, ’high’

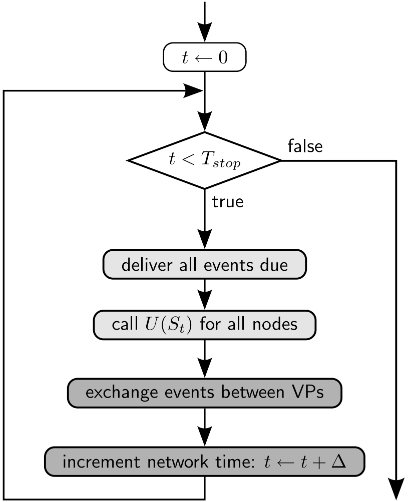
A FULL EXAMPLE

```python
import nest                                     # import NEST module
neuron = nest.Create('iaf_psc_exp')             # create a neuron
voltmeter = nest.Create('voltmeter')            # create a voltmeter
spikegenerator = nest.Create('spike_generator') # create a spike generator
nest.SetStatus(spikegenerator, {'spike_times': [10., 50.]}) # let it spike

# connect spike generator and voltmeter to the neuron
nest.Connect(spikegenerator, neuron, syn_spec={'weight' : 1E3})
nest.Connect(voltmeter, neuron)

nest.Simulate(100.) # run the simulation

# read out recording time and voltage from voltmeter and plot them
times = nest.GetStatus(voltmeter)[0]['events']['times']
voltage = nest.GetStatus(voltmeter)[0]['events']['V_m']
pl.plot(times, voltage)
pl.xlabel('time (ms)'); pl.ylabel('membrane potential (mV)')
pl.show()
```

A FULL EXAMPLE



SIMULATION LOOP



$t \leftarrow 0$

$t < T_{stop}$

false

true

deliver all events due

call $U(S_t)$ for all nodes

exchange events between VPs

increment network time: $t \leftarrow t + \Delta$

- Simulation starts at $t = 0$
- We simulate for T_{stop} ms
- $U(S_t)$ propagates the neuron state S to time t
- VPs are virtual processes
- Δ is the minimal delay in the network

☐ parallel on all threads

▨ parallel on all processes

NETWORK UPDATE

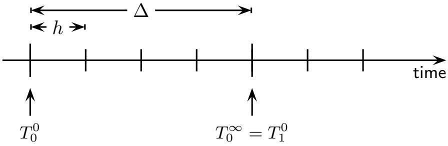
- Neurons and devices are updated in the order of their creation

- During the run of the update function, all previous events are taken care of, and new events are created
- Spikes are buffered for local and remote delivery in the next time slice
- All other events are delivered immediately to local nodes

- Devices for stimulation and recording are replicated on each VP, which also deliver locally

NODE UPDATE

During an interval of the minimal transmission delay in the network (Δ), neurons are effectively decoupled.



- The update function of nodes (U) is called every Δ steps
- The nth time slice of length Δ starts at $T_n^0 = n \cdot \Delta$ and ends at $T_n^\infty = (n+1) \cdot \Delta$
- Internally, nodes use a time step of h (e.g. for solvers)

STRUCTURED NETWORKS USING TOPOLOGY

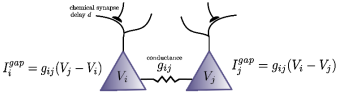
- **Invoke the topology module:**

  `from nest import topology`
- **Functionality:**
  - Set node positions on grids or arbitrary points in space (1D,2D,3D)
  - Nodes can be neurons or combinations of neurons and devices
  - Connect nodes in a position- and distance-dependent manner
  - Set boundary condition (periodic or not)
  - Enable/disable self-connections (autapses) or multiple connections (multapses)
- **Further reading:**

  `www.nest-simulator.org/documentation`

  → NEST user manual → Topological connections

GAP JUNCTIONS: IMPLEMENTATION

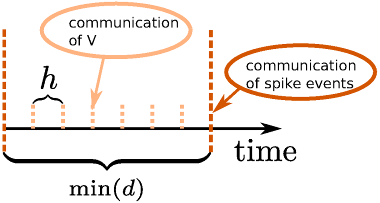


Neuron i (hh_psc_alpha_gap)

$$y_i'(t) = f_i(y_i(t)) \;,\; y_i(t_0) \text{ given}$$

$$\frac{V_i'}{C_m} = -I_i^{ionic}(V_i, m_i, h_i, n_i, p_i) + I_i^{applied}(I_i^{ex}, I_i^{in}) + I_i^{gap}(V_i, V_j)$$

- at each time point neuron i needs membrane potential of neuron j
- large system of differential equations
- naïve: communication of V in each step
- better: Jacobi waveform relaxation

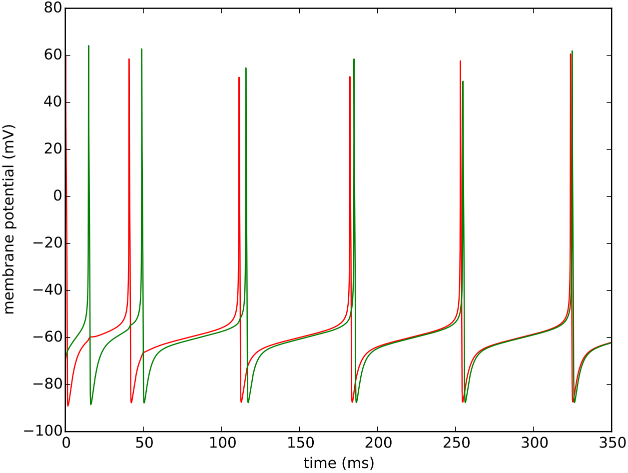


Hahne et al. (2015). A unified framework for spiking and gap-junction interactions in distributed neural network simulations. Frontiers in Neuroinformatics. 9:22

GAP JUNCTIONS: EXAMPLE

```
nest.SetKernelStatus({'max_num_prelim_iterations': 15,
                      'prelim_interpolation_order': 3,
                      'prelim_tol': 0.0001})

neuron = nest.Create('hh_psc_alpha_gap', 2, {'I_e': 100.})
nest.SetStatus([neuron[0]], {'V_m': -10.})
vm = nest.Create('voltmeter', { 'interval': 0.1})

syn_dic = {'model': 'gap_junction', 'weight': 0.5}
nest.Connect(neuron, neuron, syn_spec=syn_dic)
nest.Connect(vm, neuron)

nest.Simulate(351.)

vm_dict = nest.GetStatus(vm, 'events')
times_vm = vm_dict[0]['times']
V_vm = vm_dict[0]['V_m']
```

GAP JUNCTIONS: EXAMPLE



PARALLELIZATION IN NEST

Model developers and users (mostly) don't have to care about parallelization.

- A neuron n is created on the virtual process p, where

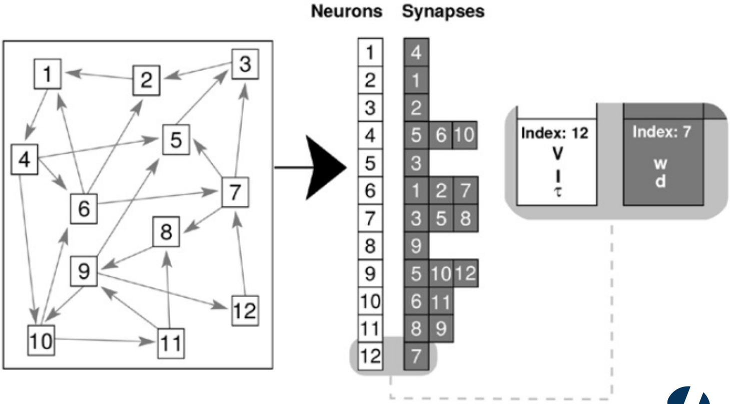
$$\mathrm{gid}(n) \mod \mathrm{N}_{\mathrm{MPI}} == p$$

- On all other VPs, a light-weight proxy is created
- Devices are replicated on each VP to distribute load

- There is one random number generator (RNG) per thread
- In addition, there is a global RNG that is kept synchronized

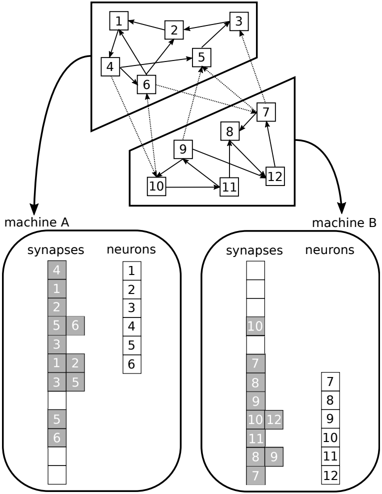
REPRESENTATION OF NETWORK STRUCTURE: SERIAL

- Each neuron and synapse maintains its own parameters
- Aynapses save the index of the target neuron



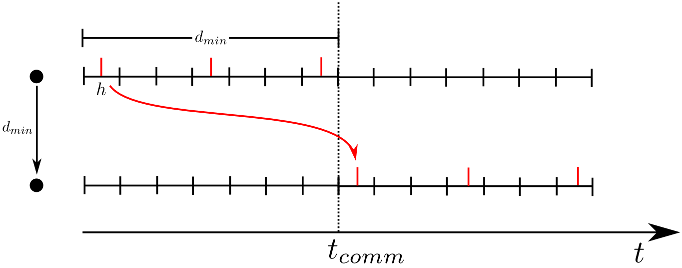
REPRESENTATION OF NETWORK STRUCTURE: DISTRIBUTED

- neurons are distributed round robin onto processes
- one target list for every neuron on each machine
- synapse stored on machine that hosts the target neuron
- wiring is a parallel operation



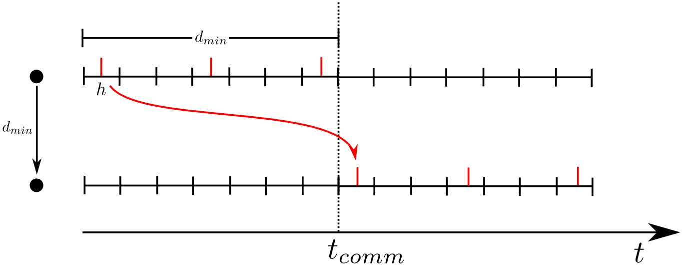
COMMUNICATION OF EVENTS

- communication only required in intervals of the minimal delay between neurons



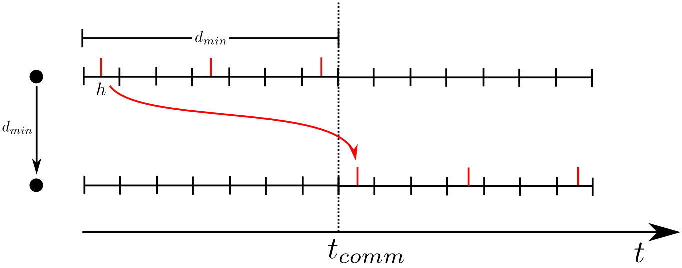
COMMUNICATION OF EVENTS

- communication only required in intervals of the minimal delay between neurons
- communication frequency independent of step size h



COMMUNICATION OF EVENTS

- communication only required in intervals of the minimal delay between neurons
- communication frequency independent of step size h
- less communications containing more data is more efficient due to overhead of communication between machines



COMMUNICATION OF EVENTS

- communication only required in intervals of the minimal delay between neurons
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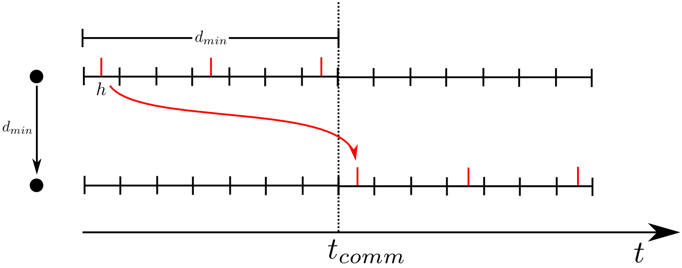
- less communications containing more data is more efficient due to overhead of communication between machines
- buffer sent to all machines (MPIAllgather)



EVENT-DRIVEN VS. TIME-DRIVEN

Event-driven simulation:

- Visit a neuron only when it receives an event (e.g. a spike)
- From $y(t_i)$, calculate $y(t_{i+1})$

Time-driven simulation:

- Visit each neuron in each time step h
- From $y(ih)$, calculate $y([i+1]h)$

EVENT-DRIVEN VS. TIME-DRIVEN

	Event-driven	Time-driven
Pros	more efficient for low input rates ’correct’ solution for invertible neuron models	more efficient for high input rates works for all neuron models scales well
Cons	only works for neurons with invertible dynamics event queue does not scale well	only ’approximate’ solution even for analytically solvable models spikes can be missed due to discrete sampling of membrane potential

EVENT-DRIVEN VS. TIME-DRIVEN

NEST uses a hybrid approach to simulation

- input events to neurons are frequent: time-driven algorithm
  - If the dynamics is nonlinear, we need a numerical method to solve it, e.g.:
    - Forward Euler: $y([i+1]h) = y(ih) + h \cdot \dot{y}(ih)$
    - Runge-Kutta (kth order)
    - Runge-Kutte-Fehlberg with adaptive step size
    - ...

  → Use a pre-implemented solver, for example, from the GNU Scientific Library (GSL).

  - If the dynamics is linear (e.g. LIF or MAT), we can solve it exactly.

EVENT-DRIVEN VS. TIME-DRIVEN

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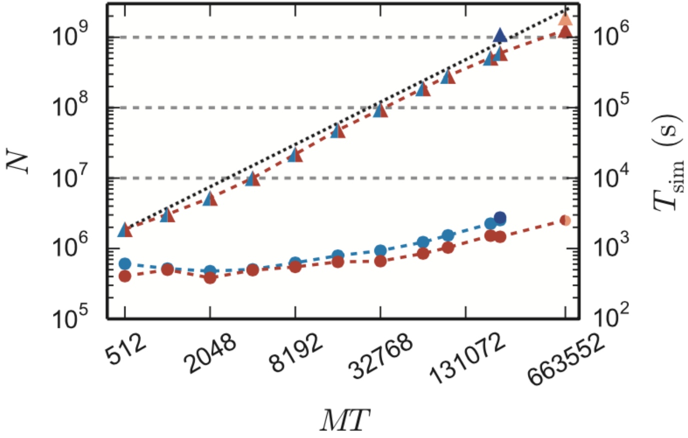
        - . . .

    → Use a pre-implemented solver, for example, from the GNU Scientific Library (GSL).

    - If the dynamics is linear (e.g. LIF or MAT), we can solve it exactly.
- events at synapses are rare: event driven component
    - Exception: gap junctions

NEST PERFORMANCE



Maximum network size and corresponding run time as function of number of virtual processes on the K computer (red) and JUQUEEN (blue). Taken from Kunkel et al., (2014), Front Neuroinf. DOI: 10.3389/fninf.2014.00078

REFERENCES AND FURTHER READING

- The NEST Initiative homepage at www.nest-initiative.org

- Gewaltig et al. (2012) NEST by example: An introduction to the neural simulation tool NEST. doi:10.1007/978-94-007-3858-4_18
- Hanuschkin et al. (2010) A general and efficient method for incorporating precise spike times in globally time-driven simulations. doi:10.3389/fninf.2010.00113
- Kunkel et al (2012) Meeting the memory challenges of brain-scale network simulation. doi:10.3389/fninf.2011.00035

Please tell us about problems. We only can fix what we know of!

NEST CONFERENCE 2019

June 24-25 2019
Norwegian university of life sciences, Ås, Norway

NEST users an developers come together to discuss

- Current research carried out with NEST
- Poster session for presenting own work
- Future development directions for NEST

Save the date!

ACKNOWLEDGMENTS

This presentation is based on previous work by many people.

- Hannah Bos
- David Dahmen
- Moritz Deger
- Jochen Martin Eppler
- Espen Hagen
- Abigail Morrison
- Jannis Schuecker
- Johanna Senk
- Tom Tetzlaff
- Sacha van Albada