

Brain Research Applications on Minsky

OpenPOWER Academia Discussion Group Workshop 2017

Andreas Herten, Forschungszentrum Jülich, 10 November 2017 *Handout Version*

Brain Research

History

Today's Challenges

Human Brain Project

HBP Pilot Systems

Motivation

JURON

Eurohack

Applications

TVB-HPC

Arbor

PLI ICA

Others

- Forschungszentrum Jülich, Germany
- Jülich Supercomputing Centre
- POWER Acceleration and Design Centre
- Strong connection to neuroscience (HPCNS)



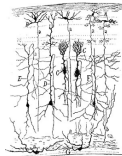
History of Brain Research

A long way down

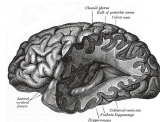
- 1700 BC: Already Egyptians had some knowledge about brain structure
- 17th c.: *Neurology*, status of brain: Thomas Willis (et al)
- 19th c.: Visualization, *neuron doctrine*: Golgi → Ramón y Cajal
- Late 19th c.: neuron electrically excitable
- 20th c.: Brodmann areas (1909); Hodgkin-Huxley model (1952); *neuroscience*
- Today: Brain still not fully decoded
 - Brain atlases in high resolution
 - Models to describe dynamic behavior
 - **Large-scale efforts**



Willis (1664)



Ramón y Cajal (1888)



Gray and Lewis (1918)

Brain Research Applications on Minsky

Brain Research

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A long way towards understanding of features of the brain

- Egyptians: Drilling hole into skull to cure headaches; brain damage
- Willis: Detailed anatomy of the brain, *Cerebri anatome: cui accessit nervorum descriptio et usus* with detailed drawings; *neurology*
- Cajal uses method of staining brains developed by Golgi (silver chromate) to visualize fibres; start of neural doctrine (=neurons are functional unit of brain)
- Late 19th century: Experiments find that the neuron is electrically excitable
- Brodmann defines areas to create atlas of responsibilities (still used today); Hodgkin-Huxley develop model to describe neurons as electrical circuits with help of giant squid (*action potential*); *neuroscience* is done

Today's Brain Challenges

A high complexity

- Many **neurons**: $\mathcal{O}(10^{11})$
- Many **connections**: $\mathcal{O}(10^4)$ synapses per neuron
- **Multi-scale** behavior
 - Molecular level
 - Cellular level
 - Brain regions
 - Whole system
- **Power** efficiency
 - Whole human brain: 30 W
 - Simulation: entire supercomputer to model small region
- Complex **data** collection



Frackowiak and Markram (2015)

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Brain Research

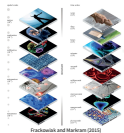
Today's Challenges

Today's Brain Challenges

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- There are many neurons
 - There are many connections between for neuron
- There are many many connections in total
- Different effects for different biological scales: zooming in reveals new features; just like in physics
 - Brain runs on amazingly low power footprint
 - Data collection is very complex: (some) dynamic studies only with large apparatus; static, but high-res studies only post-mortem, and even then is brain a complex 3D structure

Human Brain Project

HBP as a flagship



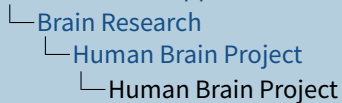
Human Brain Project

- 1 Billion € (co-funded EC and national), 10 year endeavor, *2013
- *Future and Emerging Technologies* flagship of European Commission (Horizon 2020)
- 12 sub-projects, covering multiple scales and technologies (SP7: HPC)
- Specific Grant Agreement 1 (2016 - 2018): 114 participants
- **Goal:** Build integrated ICT infrastructure to enable global collaborative effort towards understanding human brain, ultimately emulate its computational capabilities



→ <https://www.humanbrainproject.eu/>

Brain Research Applications on Minsky



Human Brain Project

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→ <https://www.humanbrainproject.eu/>

To understand (*decode*) such a complex organ is an endeavor which needs a large-scale effort → EU Flagship Project

- Funding: 50 % from EU, 50 % from partners
- Sub-projects which focus on different kinds of efforts (mouse brains, theoretical, neuromorphic computing, ..., even robotics!)
- Current: Specific Grant Agreement 1

HBP Pilot Systems

- Measuring and simulating brain components: computational intensive!
- High Performance Analytics and Computing Platform (HPAC)

Brain Research Applications on Minsky

└ HBP Pilot Systems

└ Motivation

└ HBP & Supercomputers

HBP & Supercomputers

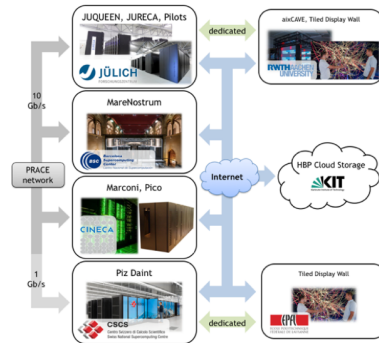
- Measuring and simulating brain components: computational intensive!
- High Performance Analytics and Computing Platform (HPAC)

- Already now, HBP needs many computing resource for all the simulations and measurements
→ HPAC
- But simulations will get more and more sophisticated, so demand only increases
- With that large performance need: Special requirements to supercomputers identified
- PCP new way of EU to involve vendors into procurement

HPAC Platform

High Performance Analytics and Computing

- HPC and data infrastructure services
Currently: loosely coupled, not yet federated
- Current components
 - Supercomputers at BSC (MareNostrum 4), CINECA (Pico, MARCONI), CSCS (Piz Daint), JSC (JUQUEEN, JURECA, Pilots)
 - Cloud services at KIT
 - Visualization services at RWTH and EPFL



Brain Research Applications on Minsky

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HPAC Platform

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- Largest European supercomputers bundled
- Eventually coupled together
- Currently on the way there, with individual parts finished (collaboratory, UNICORE)

- Measuring and simulating brain components: computational intensive!
- High Performance Analytics and Computing Platform (HPAC)
- Large-scale brain simulations: PFLOP/s, PB
 - Need capability of a supercomputer!
- Special requirements
 - Interactive, scalable visualization (in-situ)
 - Large memory footprint of data (dense memory, fast interconnects)
 - Dynamic resource management, interactive steering
 - Various data sources (eventually: federated services)
- Pre-Commercial Procurement of two systems: **JULIA** and **JURON**



JULIA

- Cray (CS-Storm)
- 60 nodes, each 1 Intel Xeon Phi KNL
- OmniPath network

JURON

- IBM-NVIDIA (Minsky)
- 18 nodes, each 2 P8', 4 P100, NVMe SSDs
- InfiniBand EDR

Common local storage



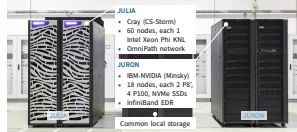
JULIA & JURON: Human Brain Project *Prototypes*

Brain Research Applications on Minsky

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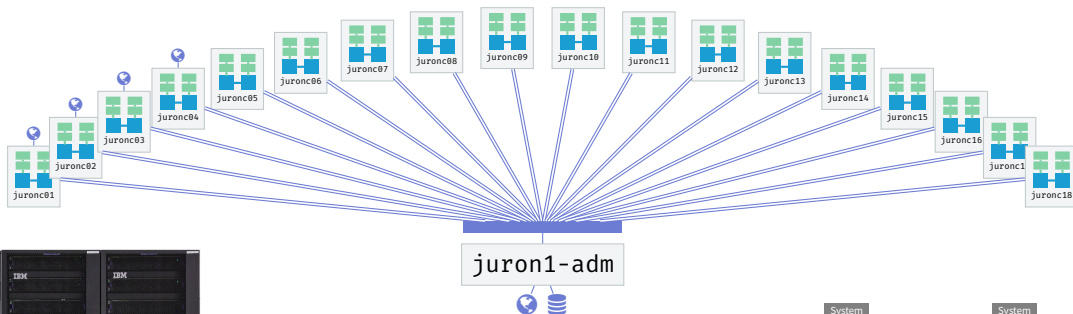
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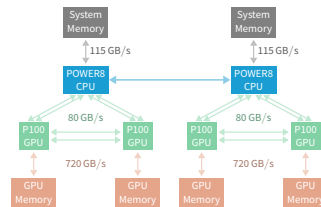
- Two system: Intel-KNL-based JULIA and POWER8'-P100-based JURON
- Match requirements in their own ways
- Middle: A common storage cluster, attached to JURON and JULIA faster than Jülich's global file system GPFS

System Configuration



- JURON = Juelich + Neuron
- ≈ 350 TFLOP/s peak (double)
- Memory

Technology	Capacity / TB	Bandwidth / TB/s
HBM2	1.1	52
DDR4	4.5	4.1
NAND flash	28	0.05



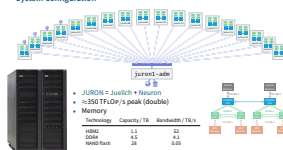
Brain Research Applications on Minsky

└ HBP Pilot Systems

└ JURON

└ System Configuration

System Configuration



- JURON's 18 compute nodes, connected via Ethernet and InfiniBand to switch; login node connected via Ethernet to switch
- Login node: access from outside and to Jülich storage resources (+ PCP storage system)
- Also: 4 visualization nodes with direct access from outside
- Capacity and bandwidth are combined values

GPU Hackathon in Jülich

First HBP Applications on JURON

- Eurohack: 1 week of application porting to GPU at JSC in March 2017
 - 10 teams; 3 neuroscience
 - Arbor Optimizing GPU code of simulation (formerly *NestMC*)
 - TVB-HPC First port of back-end to CUDA
 - The PLI Guys Build CUDA back-end to Python simulation
 - >1000 jobs launched, $\frac{2}{3}$ on JURON
 - Every team accelerated code and went home motivated
- Strong interest in GPU and JURON



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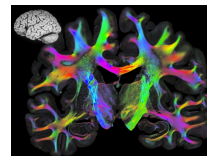
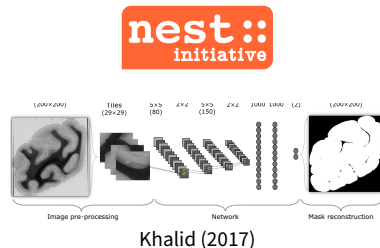
- GPU Hackathon (*Eurohack*) in Jülich; one of the events organized with ORNL all over the world
- Intense work atmosphere, very productive
- Three applications from neuroscience, in the following presented as examples

Applications

Diverse Set of Applications

Many scales, many steps

- Simulation
 - Regions: **The Virtual Brain**
 - Neural networks: **Nest**
 - Neurons with compartments: **Arbor**, Neuron
- Measurement
 - Coupling of data
 - Electrophysiology
- Post-processing
 - **Post-processing** of scanned data
 - Automated stitching
 - Matching of images taken with different methods



Axer (2017)

Brain Research Applications on Minsky

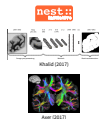
└ Applications

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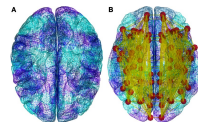
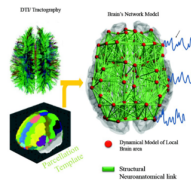
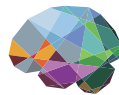
- Jülich specializes in tools for simulation and post-processing of scanned data
- Strong connection with Supercomputing Centre, specialized interface division: High Performance Computing in Neuro Science (HPCNS) + Simulation Lab Neuro Science (SLNS)
- There's much more to it – 12 sub-projects of HBP

Applications

TVB-HPC

- Framework for simulation of brain **dynamics** on large scale [6]
 - Biologically realistic connectivity matrix (*connectome*)
 - Neural mass models, sparse matrix linear solution (60 - 1000 elements), several free parameters
 - Models built on top of clinical data (fMRI, ...)
 - Goal: Help patients with neurological disorders, compare brain
- Current software stack
 - Python simulation core, expendable by Matlab scripts
 - Web-based visual control center
 - Domain-Specific Language to describe brain models (*IDLE*)

→ <http://www.thevirtualbrain.org/tvb/>



Brain Research Applications on Minsky

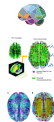
└ Applications

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└ The Virtual Brain

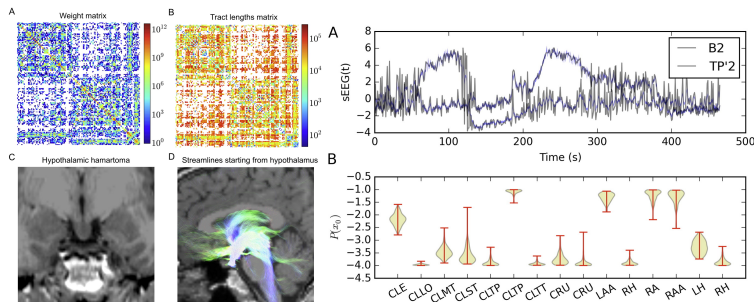
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- TVB: software infrastructure to simulate individual brains as models
- Match with measurements; structural vs. functional data
- Eventual goal: simulate a patient's brain in software and guide cure for illness
- Basically written in Python with interfaces to individual Matlab scripts for extension
- View the virtual brain at a web-based applications
- DSL for description of brain models
- Pictures
 1. Logo TVB
 2. Flow of typical brain simulation; input are fibre structures (up, connectome, visualized for example with *Diffusion Tensor Imaging*) and regions of brain
 3. Connectome close-up

Example TVB Science on JURON



- Recently run: Monte Carlo model inference for clinical epilepsy models
Pictures from “The Virtual Epileptic Patient: Individualized whole-brain models of epilepsy spread” [7]
- Currently single-threaded application; no performance gain yet

Brain Research Applications on Minsky

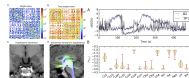
└ Applications

└ TVB-HPC

└ Example TVB Science on JURON

- Also TVB currently runs on JURON
- Example epileptic simulation

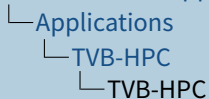
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- Traditional approach: Serial computation of models
- TVB-HPC: Fast, parallel back-end (parallel in parameters)
- At GPU hackathon:
 - Optimize specific mass, coupling, post-processing models
 - Study data access issues
 - Learn advanced GPU techniques
 - 20× speedup
- **JURON**: CUDA code for *Kuramoto* model as proof-of-concept
- Since then: Automated code generation

Brain Research Applications on Minsky



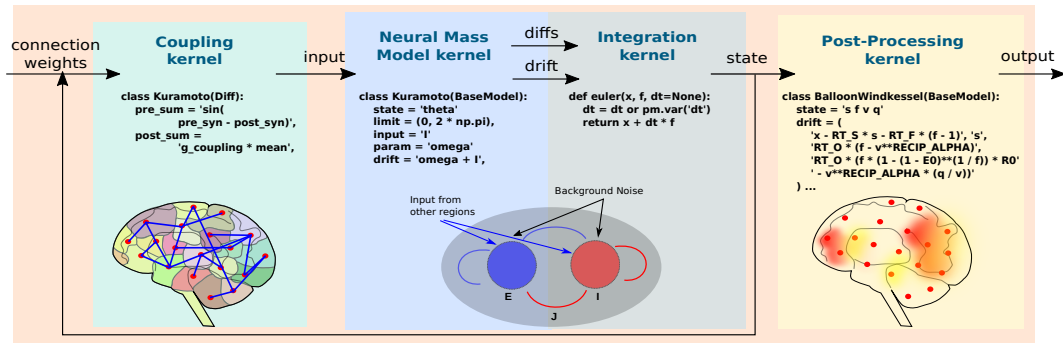
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- JURON: CUDA code for Kuramoto model as proof-of-concept
- Since then: Automated code generation

- TVB: Serial simulation of single brain model
- TVB-HPC: Optimized, HPC-targeted simulation of multiple versions of model by simulating many parameters of model at once in parallel
 - First (and at Hackathon): One single model ported to CUDA – very good results
 - Now: Focus on automated code generated

Code Generation in TVB-HPC

Targeting different accelerators



S. Diaz (2017)

- DSL for models (types, dimensions, flow, dependencies)
- Generate parameter-parallel code with `loo.py`; back-ends: CUDA, OpenCL, Numba, C

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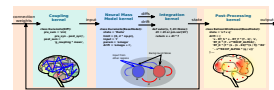
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└ Code Generation in TVB-HPC

Code Generation in TVB-HPC

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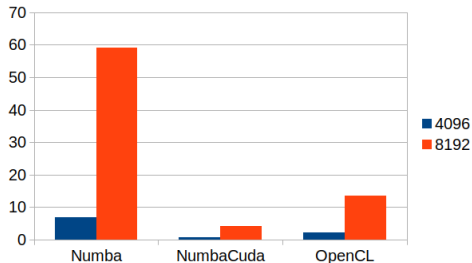


- DSL for models (types, dimensions, flow, dependencies)
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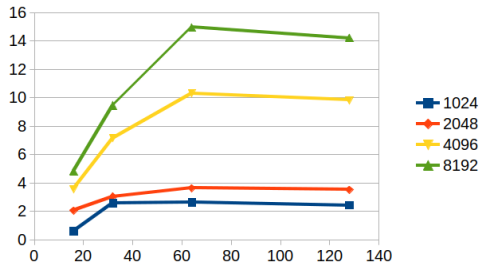
- User writes models in DSL
- Models are most of the time neural mass models, but also coupling and integration kernels (or select one pre-existing for the latter)
- From DSL, `loo.py` is used to generate to-be-accelerated code

Code Generation in TVB-HPC

Results on JURECA



Test kernel execution time (y/ms) for different targets



Test kernel execution time speedup Numba+CUDA vs. Numba (y) for different number of threads (x)

- JURECA node: 2 Intel Haswell CPUs (12 cores), 2 NVIDIA Tesla K80 GPUs
- **Numba**: Decorator-based auto-acceleration for Python (JIT compilation with `@jit`); different targets

Generated CPU-targeted code

```
@lpy_numba.jit
def loopy_krnl(n, nnz, row, col, dat, vec, out):
    for i in range(0, -1 + n + 1):
        jhi = row[i + 1]
        jlo = row[i]
        for k in range(0, -1 + n + 1):
            acc_j = 0
            for j in range(jlo, -1 + jhi + 1):
                acc_j = acc_j + dat[j]*vec[col[j]]
            out[i] = k*acc_j
```

Generated GPU-targeted code

```
@ncu.jit
def loopy_krnl_in(n, nnz, row, col, dat, vec, out):
    if -1 + -512*bIdx.y + -1*tIdx.y + n >= 0 and -1
    ↪ + -512*bIdx.x + -1*tIdx.x + n >= 0:
        acc_j = 0
        jhi = row[1 + tIdx.x + bIdx.x*512]
        jlo = row[tIdx.x + bIdx.x*512]
        for j in range(jlo, -1 + jhi + 1):
            acc_j = acc_j + dat[j]*vec[col[j]]
        out[tIdx.x + bIdx.x*512] = (tIdx.y +
        ↪ bIdx.y*512)*acc_j
```

S. Diaz (2017)

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Brain Research Applications on Minsky

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└ TVB-HPC

└ Code Generation in TVB-HPC

Code Generation in TVB-HPC

Results on JURECA

Generated CPU-targeted code

```

@jit
def loopy_kernel(x, m2, row, col, dst, src, out):
    for i in range(0, -1 - m + 1):
        [m] = row[i - 1]
        [m] = row[i]
        for k in range(0, -1 - m + 1):
            out[i] = m
    out[i] = m

```

Generated GPU-targeted code

```

@jit
def loopy_kernel(x, m2, row, col, dst, src, out):
    if -1 - m2 - m2 < 0:
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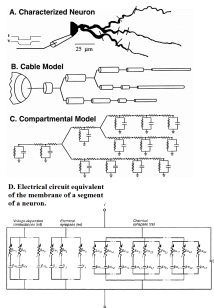
1 / 10 (100%)

- Current studies with loop.py generation on JURECA, but code runs also on JURON
- Up to 16-fold speed-up for Numba+CUDA vs Numba
- In Numba+CUDA, Numba generates CUDA code in run-time; also here loop.py provides the raw code, which is more targeted towards CUDA already

Applications

Arbor

- TVB: Large scale; effective models; dynamics
- Nest: Biologically correct; point-like neurons; large, spiking networks
- Arbor: Neurons with internal structure, multi-compartment



- Hodgkin-Huxley model: network of neurons as circuit [3]
- Neuron: axonic delay, synaptic functions, tree of cables connecting to body
- Cables: electrical compartments (resistance, capacitance)

$$\frac{\partial}{\partial x} \left(\sigma \frac{\partial v}{\partial x} \right) = \left(c_m \frac{\partial v}{\partial t} + r_m(v - e^{\text{rev}}) + \sum_{\text{channels } k} g_k(v, t)(v - e_k^{\text{rev}}) \right) \cdot \frac{\partial S}{\partial x} + \sum_{\text{synapses } k} I_k^{\text{syn}}(v, t)\delta_{x_k} + \sum_{\text{injections } k} I_k^{\text{inj}}(t)\delta_{x_k}$$

→ Neuron is (band) matrix based on known conductance

Brain Research Applications on Minsky

Applications

Arbor

Arbor Introduction

Arbor Introduction

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- Hodgkin-Huxley model: network of neurons as circuit [3]
- Neuron: axonic delay, synaptic functions, tree of cables connecting to body
- Cables: electrical compartments (resistance, capacitance)

$$\frac{d}{dt} \begin{pmatrix} V \\ \mathbf{m} \\ \mathbf{h} \\ \mathbf{n} \end{pmatrix} = \begin{pmatrix} -\frac{1}{\tau_m} V + \frac{1}{\tau_m} \sum_{i=1}^N g_i (V_i - V) \\ \sum_{i=1}^N g_i (V_i - V) \\ \sum_{i=1}^N g_i (V_i - V) \\ \sum_{i=1}^N g_i (V_i - V) \end{pmatrix} \frac{dV}{dt}$$

→ Neuron is (band) matrix based on known conductance

- Zoom in to brain: TVB → Nest → Arbor
- Nest looks at really large networks of point-like neurons and simulates spikes
- Arbor includes now also the internal structure of neurons (neurons are multi-compartment)
- A simplified neuron sketch: Neuron is core, which connects through long axons to the synapses, which are attached to dendrites, of other neurons
- With that a tree of cables is created, first seen by Hodgkin and Huxley
- Cables can be described as partial differential equations of capacitance and resistance
- Describing all cables and further structures leads to a sparse matrix, which has most entries on the main band (but not all)

- Aim: Real-time, morphologically detailed, large-scale simulations
- Optimized for modern HPC systems (parallelism, accelerators)
- Easy to integrate, easy to extend
- Collaboration of JSC, CSCS, BSC
- Open Source Software, modern development methods
- C++, CUDA, Intel Thread Building Blocks, HPX

→ <https://github.com/eth-cscs/arbor>

Brain Research Applications on Minsky

└ Applications

└ Arbor

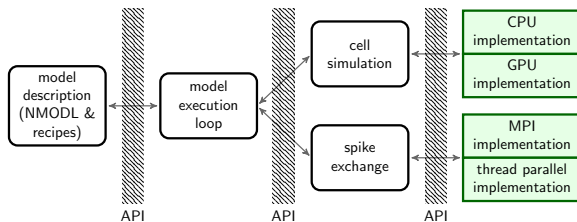
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- Easy to integrate, easy to extend
- Collaboration of JSC, CSCS, BSC
- Open Source Software, modern development methods
- C++, CUDA, Intel Thread Building Blocks, HPX

→ <https://github.com/eth-cscs/arbor>

- Other simulators have long history in development and grew historically; → not a-priori well-suited for HPC-like simulations (which are needed to eventually simulate the real brain)
- Arbor effort of JSC, CSCS, BSC to develop a modern simulator, which is built with HPC in mind directly (Arbor was previously called NestMC)
- Open Source Software, developed on Github, Continuous Integration
- Many modern technologies



- **Modular:** Substitute models with internal API
- Modeling language: **NMODL** (Neuron) \Rightarrow generate hardware-specific code
- Communication: MPI (global), Intel TBB or C++11 Threads (local threads)
- Backends: CUDA, AVX512, AVX2
- **GPU back-end** available
 - Hackathon project: Optimize sparse matrix computation on GPU
 - Solution: Use padding $\rightarrow 3\times$ to $10\times$ speedup

Applications

- Arbor

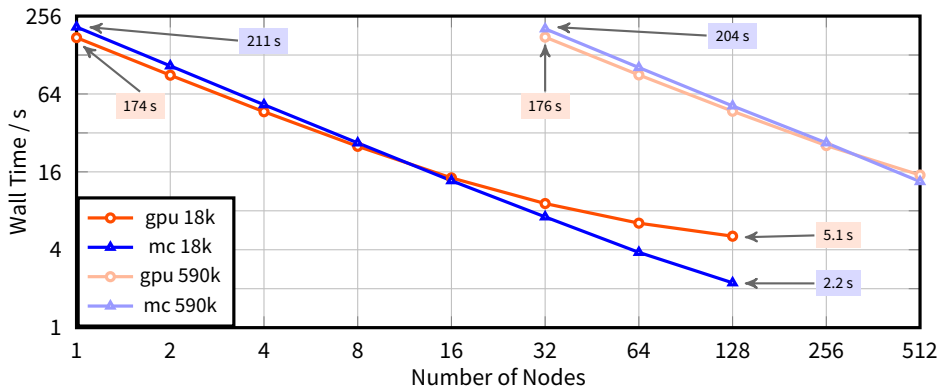
-Architecture of Arbor

- **Modular:** Substitute models with internal API
- **Modeling language:** **NMODL** (Neuron) \Rightarrow generate hardware-specific code
- **Communication:** MPI (global), Intel TBB or C++11 Threads (local threads)
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- **GPU back-end available**
 - Hackathon project: Optimize sparse matrix computation on GPU
 - Solution: Use padding \Rightarrow 3x to 10x speedup

- Adopts NEURONS modeling language (NEURON: Another multi-compartment simulator, but also not well-suited for parallel execution w/o modifications)
- Can target GPUs and Xeon Phi (KNLs)
- CPU sorts and packages data closely together, package potentially offloaded to accelerator, solved, and back

Current Status

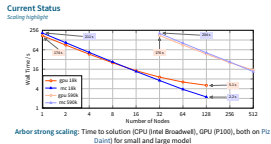
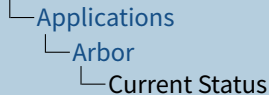
Scaling highlight



Graph by Ben Cumming

Arbor strong scaling: Time to solution (CPU (Intel Broadwell), GPU (P100), both on **Piz Daint**) for small and large model

Brain Research Applications on Minsky

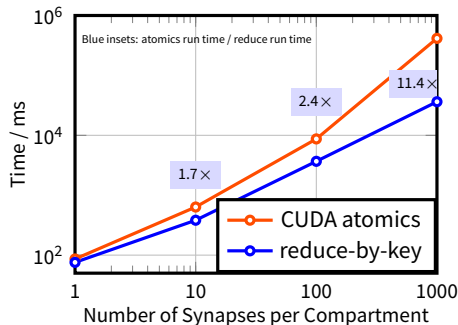


- Currently no JURON plots available, but same/similar tests have been run
- Plot on Piz Daint (which also has P100 GPUs)
- Still more potential within GPUs, actively developed
 - Small model
 - Low number of nodes is better for GPU, because then device can crunch a lot of data (which it is good at)
 - But speed-up eaten up by CPU, which needs to package the large data for the GPU
 - For high number of nodes CPU is faster because the data packages are smaller and can be solved by the CPU without any transfer overheads
 - Large model: pretty much similar

Current Status

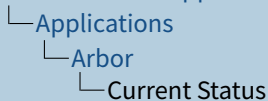
Overview

- Arbor shows good behavior in strong and weak scaling
- GPU acceleration: matrix solver (*Hines* solver); state evolution
- Specific optimizations available, targeting hardware characteristics
Example *reduce-by-key*: Prevent race conditions by warp-synchronous binary reductions
- JURON in use, no dedicated measurements yet

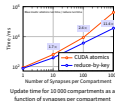


Update time for 10 000 compartments as a function of synapses per compartment

Brain Research Applications on Minsky

Current Status
Overview

- Arbor shows good behavior in strong and weak scaling
- GPU acceleration: matrix solver (Hines solver); state evolution
- Specific optimizations available, targeting hardware characteristics
Example reduce-by-key: Prevent race conditions by warp-synchronous binary reductions
- JURON in use, no dedicated measurements yet



- Much effort in developing all the details
Example: Hines solver – A solver for mostly-band-matrices; very specific
- Example: Reduce-by-key – Instead of using mutexes to write to common memory location, reduce-by-key uses warp-level binary reductions to increase memory efficiency

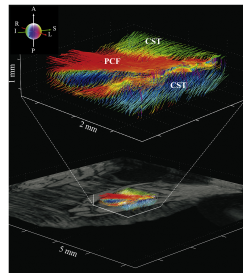
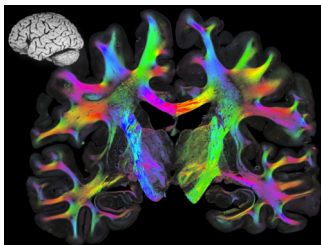
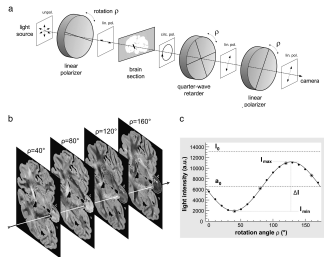
Applications

PLI ICA

3D PLI ICA

PLI...

- 3D Polarized Light Imaging (PLI): Capture brain slices under polarized light
 - Capture at many angles (18, 0° to 170°)
 - Myelin around axons refracts light based on inclination to polarization plane
- Resolve 3D structure of nerve fibers



Images by Axer et al. [8]

Brain Research Applications on Minsky

└ Applications

└ PLI ICA

└ 3D PLI ICA

3D PLI ICA

PLI...

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 - Capture at many angles (18, 0° to 170°)
 - Myelin around axons refracts light based on inclination to polarization plane
- Resolve 3D structure of nerve fibers



Copyright: Minsky et al. 2017

- Amount of transmitted light changes (sinusoidally) as function of angle between axon and polarization plane of light; actually light is polarized with filters which change the polarization plane
- Use information of refraction to measure brain in 3D (in slices)

3D PLI ICA

...ICA

- Independent Component Analysis (ICA):
Separate complex signal into components;
mixture of sources → individual
contributions
 - Signal-processing method, blind source
separation
 - Basis: Sinusoidal distribution of
measurement basis functions
- Identify noise and artifacts in decomposition
for removal

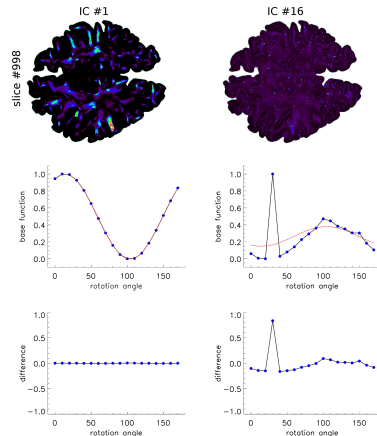


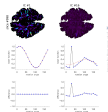
Image by Dammers et al. [9]

Brain Research Applications on Minsky

- └ Applications
 - └ PLI ICA
 - └ 3D PLI ICA

3D PLI ICA
— ICA

- Independent Component Analysis (ICA):
Separate complex signal into components;
mixture of sources → individual
contributions
- Signal-processing method, blind source
separation
- Basis: Sinusoidal distribution of
measurement basis functions
→ Identify noise and artifacts in decomposition
for removal



- ICA: Method to decompose signal
- Measured signal is overlaid mixture of unknown and independent sources; mixture on sources appear on all measurements (number of measurements needs to be greater than number of sources)
- ICA decomposes mixture into individual sources
- Picture: different decomposition parts – signal (left) vs. noise (right)
Signal fits very well to a sinus function, noise not that well. Bottom: difference to sinus fit

- **Computationally intensive** analysis
→ distribute compute and I/O
- **Large data**
750 GB per slice, 325 TB per brain
- Written in **Python**
Cython, numpy, scipy, mpi4py
- Legacy code with many parts
- **GPU Hackathon:**
 - Extract compute intensive part to C
 - Use OpenACC and CUDA for acceleration
 - Prototype-like development

```
e.kurt = stats.kurtosis(np.dot(input_data,  
↪ weights).T, axis=1, fisher=True)
```



```
#pragma acc data copyin(input_v[0:n])  
#pragma acc parallel loop reduction(+:mean)  
for(unsigned int i=0; i < n; ++i)  
    mean += input_v[i]/n;  
#pragma acc parallel loop copyin(mean)  
↪ reduction(+:variance)  
↪ reduction(+:kurtosis)  
for(unsigned int i = 0; i < n; ++i) {  
    double tmp = input_v[i] - mean;  
    variance += (tmp*tmp);  
    kurtosis += pow(tmp,4);  
}  
kurtosis /= (variance*variance);  
return (n*kurtosis-3.0);
```


Brain Research Applications on Minsky

└ Applications

└ PLI ICA

└ ICA Challenges and Status

ICA Challenges and Status

- Computationally intensive analysis
→ distribute compute and I/O
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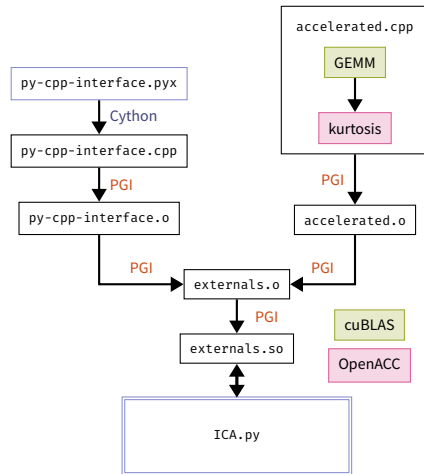
w_kurt = stats.kurtosis(np.dot(input_data,
                               ~ weights).T, axis=-1, fisher=True)
                                ↓
for npg in data.copyin(input_v[0:n])
for npg acc parallel: loop reduction(+mean)
for(assigned int i=0; i < n; ++i)
  mean += input_v[i]*w
for npg acc parallel: loop copyin(mean)
  ~ reduction(+variance)
  ~ reduction(+kurtosis)
  double tmp = input_v[i] - mean;
  variance += (tmp*tmp);
  kurtosis += pow(tmp,4);
}
kurtosis /= (variance*variance);
return (-kurtosis-1.0);

```

- ICA: Team I co-mentored at GPU hackathon
- Prototype-like development to port the Python application to GPU
- Decided not to use PyCUDA (or similar) but to write C implementations of kernels and add wrappers

ICA Results of Porting

- Hybrid Python, C, OpenACC, CUDA code
- JURON faster than JURECA
 - Data transfer: $10\times$ (H2D), $6\times$ (D2H)
 - Compute: $7\times$
- Still many parts of program CPU-only \rightarrow limited possible speed-up, data transfer overheads
- Benefit from Hackathon:
 - Create Python interface
 - Speak to experts on libraries
 - Write CUDA prototype
 - Formulate plan for future
- Unfortunately, code is currently rolled back to serial version to fix communication errors



- Hybrid Python, C, OpenACC, CUDA code

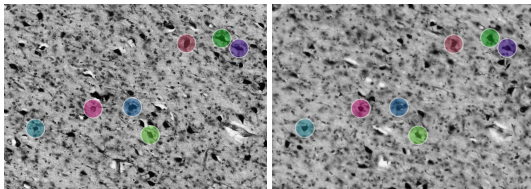
- Hybrid Python, C, OpenACC, CUDA code
- JURON faster than JUREKA
 - Data transfer: $10 \times$ (H2D), $6 \times$ (D2H)
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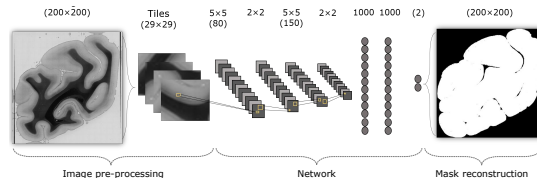
- Eventually: Hybrid code with many programming languages and programming models
- Test-run of C kernel on JURON and JURECA: JURON usually faster
- Still, many parts need to be ported to GPU to benefit from fewer memory copies
- Currently: Fixing MPI deadlock bugs in serial version

Other HBP Applications on JURON

- Only three applications highlighted (TVB-HPC, Arbor, PLI ICA)
- Many applications more on JURON!
 - 2D \rightarrow 3D image registration
 - Multi-scale brain image stitching
 - Pattern recognition



Huysegoms (2017)



Khalid (2017)

- Brain research exciting also for computational science
 - Minsky system **JURON** deployed as pilot supercomputer for Human Brain Project
 - System under intensive use (not only by HBP users)
 - TVB-HPC and Arbor: Two brain simulation applications operating on different scales
 - PLI ICA: Cleanup of scanned images
 - Many applications benefit from GPU (and also NVLink)
- HBP helps to drive development of future supercomputers

**Thank you
for your attention!**
a.herten@fz-juelich.de

Appendix

Glossary

References

Appendix

Glossary & References

- API** A programmatic interface to software by well-defined functions. Short for application programming interface. 41
- Arbor** Multi-compartment simulation of neural networks, previously called *NestMC*. 2, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 56, 57
- BSC** Barcelona Supercomputing Center, a Spanish supercomputing site. 12, 39
- CINECA** An Italian consortium of universities operating supercomputers. 12
- CSCS** The national supercomputing centre of Switzerland. 12, 39
- CUDA** Computing platform for GPUs from NVIDIA. Provides, among others, CUDA C/C++. 19, 29, 31, 33, 39, 41, 52, 54, 60

DSL A Domain-Specific Language is a specialization of a more general language to a specific domain. [31](#)

EPFL École Polytechnique Fédérale de Lausanne, Switzerland. [12](#)

JSC Jülich Supercomputing Centre, the supercomputing institute of Forschungszentrum Jülich, Germany. [12](#), [19](#), [39](#), [60](#)

JURECA A multi-purpose supercomputer with 1800 nodes at JSC. [33](#), [34](#), [54](#)

JURON One of the HBP pilot system in Jülich; name derived from Juelich and Neuron. [19](#), [27](#), [28](#), [45](#), [54](#), [56](#), [57](#)

KIT Karlsruhe Institute of Technology, Germany. [12](#)

MPI The Message Passing Interface, a API definition for multi-node computing.
41

NVIDIA US technology company creating GPUs. 33, 34, 60

NVLink NVIDIA's communication protocol connecting CPU ↔ GPU and GPU ↔ GPU with 80 GB/s. PCI-Express: 16 GB/s. 57, 60

OpenACC Directive-based programming, primarily for many-core machines. 52, 54

OpenCL The *Open Computing Language*. Framework for writing code for heterogeneous architectures (CPU, GPU, DSP, FPGA). The alternative to CUDA. 31

P100 A large GPU with the Pascal architecture from NVIDIA. It employs NVLink as its interconnect and has fast HBM2 memory. 43

Pascal GPU architecture from **NVIDIA** (announced 2016). 60

RWTH RWTH Aachen University, Germany. 12

Tesla The GPU product line for general purpose computing computing of **NVIDIA**. 33, 34

TVB-HPC High-Performance Computing sub-project of The Virtual Brain. 29, 30, 31, 32, 33, 34, 35, 56, 57

CPU Central Processing Unit. 33, 34, 43, 54, 60

GPU Graphics Processing Unit. 19, 20, 29, 33, 34, 41, 43, 45, 52, 57, 60

HBP Human Brain Project. 7, 8, 19, 56, 57, 60

ICA Independent Component Analysis. 48, 49, 50, 51, 52, 53, 54, 55, 56, 57

PLI Polarized Light Imaging. 48, 49, 50, 51, 56, 57

TVB The Virtual Brain. 25, 26, 27, 28, 37, 60

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