SCALING UP YOUR RESEARCH
SUPERCOMPUTING IN A NUTSHELL

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SUPERCOMPUTERS FOR (BRAIN) SIMULATION

An example

• Simulation:
  0.52 billion neurons
  5.8 trillion synapses
  on JUQUEEN at Jülich Supercomputing Centre:
  1s of biological time simulated in **5.2min**

• JUQUEEN: ~250,000x more compute capacity than standard quad-core processor

• Same simulation on standard computer: ~2 years
  … and the network model would not fit into memory

https://doi.org/10.3389/fninf.2018.00002
WHY TO USE A SUPERCOMPUTER?

Application requirements exceed hard drive, memory and/or compute capacity of standard computer. HPC enables larger network models or more detailed networks.

Get same results faster: Run same application multiple times with different parameters: parameter studies or parameter optimisation.

Feasibility: experiments are impossible (e.g. evolution of a galaxy).

Ethics: real-life experiments would be un-ethical (e.g. design and test of new medical devices).

Costs: real-life experiments would be too expensive (e.g. car crash tests at early design stage).
SUPERCOMPUTERS IN A NUTSHELL …

“Racks” or “cabinets” …

… each with several “node boards” or “servers”, each with multiple “nodes” …

… all connected by a high-bandwidth network…

Login nodes
Entry point from the outside

Batch system
Scheduler decides which job runs where and when

Periphery
- Storage system
- Network link to the outside world
- Archive

… each node has:
- Processors (CPUs), each often with multiple cores
- Main memory
- I/O unit (or separate I/O nodes)
- Network devices, e.g.
  - Admin network
  - High bandwidth network
- Optional: GPUs or other accelerators
BASIC PRINCIPLES TO USE SUPERCOMPUTERS

General principle
1. Divide the problem into small sub-problems
2. Distribute the sub-problems to compute units
3. Communicate results: let the compute units exchange intermediate results or other required information
4. Combine the results of the sub-problems into the global result; typically requires more communication

How is it done in NEST?
• Virtual processes (VP): POSIX threads living in MPI processes with one or multiple threads per process
• Neurons in the network are distributed among the VPs (round robin)
• If a neuron is connected to a neuron handled by another VP, the spikes are sent to the other VP using MPI and OpenMP

SUPERCOMPUTING AND THE HUMAN BRAIN PROJECT

- HBP is a Future and Emerging Technologies (FET) Flagship project co-funded by the European Union with a total duration of 10 years and up to 1 billion € funding
- >100 partner institutions from 20 European countries

Goals for 10 year endeavor

- Build a European Research Infrastructure (RI) for the neuroscience community:
  - Six Platforms: Neuroinformatics, Brain Simulation, High Performance Analytics and Computing, Medical Informatics, Neuromorphic Computing, Neurorobotics
- Gather, organise and disseminate data describing brain and its diseases
- Simulate the brain
- Build multi-scale scaffold theory and models for the brain
- Develop brain-inspired computing, data analytics and robotics.
Build and operate a supercomputing, data and visualization infrastructure enabling scientists to

- Run large-scale, data intensive, interactive brain simulations
- Manage the large amounts of data used and produced in the HBP
- Manage complex workflows comprising concurrent simulation, data analysis & visualization workloads
SUPERCOMPUTING IN THE HBP
HPAC PLATFORM: UNIFIED ACCESS TO RESOURCES

HBP Collaboratory
Interactive visualisation
Command line

Middleware: unified access to resources
HOW TO GET ACCESS TO SUPERCOMPUTERS?

Pilot systems of the Human Brain Project

- Two supercomputer pilots, developed by Cray and IBM-NVIDIA
- Architecture design tailored for neuroscience applications and driven by HBP use cases
- Cutting-edge technology
- JULIA: Xeon Phi (Knights Landing; KNL)
- JURON: Power8 and NVIDIA Tesla P100
- Accessible as part of the HPAC Platform

Info: https://trac.version.fz-juelich.de/hbp-pcp/wiki/Public
HOW TO GET ACCESS TO SUPERCOMPUTERS?

Standard way: proposal-based access for projects

- Supercomputers are expensive resources shared by multiple research communities
- Resource distribution based on technical feasibility and scientific excellence: peer-reviewed proposals
  1. Write a proposal: scientific plan, technical details of the application/workflow (scaling behaviour)
  2. Proposal is reviewed technically by HPC site, scientifically by independent experts
  3. Computing time allocation is granted for typically one year
- No fee for supercomputer usage
- National and European (PRACE) calls
HOW TO GET ACCESS TO SUPERCOMPUTERS?

Help needed? Preparatory Access – Support from the Simulation Labs

Jülich Supercomputing Centre and PRACE offer Preparatory Access

- Lightweight application process, call open throughout the year
- Small amount of computing time, accompanied by support from the JSC Simulation Labs or PRACE experts, respectively

Expertise offered by the SimLabs at JSC

- Porting and tuning of codes
- Performance analysis and scaling improvement of codes or applications
- (Re-) design of computational methods needed to exploit highly parallel architectures
- Members of SimLab Neuroscience are experienced NEST developers

SimLab Neuroscience
Lead: Prof. Dr. Abigail Morrison
Contact: slns@fz-juelich.de
HOW TO GET ACCESS TO SUPERCOMPUTERS?

A summary

Model is too large for standard PC, but large supercomputer is not needed

Pilot systems at JSC

Simulation of large model

Apply for project allocation

No experience yet with HPC, need help to get started

Apply for preparatory access
| Human Brain Project | www.humanbrainproject.eu  
|---------------------|-------------------------|
|                     | @HumanBrainProj  
|                     | Human Brain Project  
|                     | http://www.youtube.com/user/TheHumanBrainProject  
|                     |  
| HBP HPAC Platform   | https://hbp-hpc-platform.fz-juelich.de/  
|                     | @HBPHighPerfComp  
|                     | hpac-support@humanbrainproject.eu  
| SimLab Neuroscience  | http://www.fz-juelich.de/ias/jsc/slns/  
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