Towards a high performance analytics and computing platform for brain research

D. Pleiter | San Jose | 5 April 2016
Overview

- Introduction to Jülich Supercomputing Centre and Human Brain Project
- Selected objectives of the Human Brain Project
- Interactive supercomputing and future supercomputer requirements
- Conclusions
Jülich Supercomputing Centre

Provisioning of HPC infrastructure

- HPC resources for
  - Regional and national level
  - Europe (PRACE, EU projects)
- Application support

Education and Training

Research and development

- Computational science: SimLab
- Algorithms, performance analysis and tools
- HPC architectures and technologies
  - Exascale Laboratories
  - Community data management services
HPC Infrastructure at JSC: Dual Track Concept

IBM Power 4+ JUMP, 9 TFlop/s

IBM Power 6 JUMP, 9 TFlop/s

Intel Nehalem JUROPA 300 TFlop/s

Intel Haswell JURECA ~ 2 PFlop/s

+ Booster ~ 10 PFlop/s

General-Purpose Cluster

IBM Blue Gene/L JUBL, 45 TFlop/s

IBM Blue Gene/P JUGENE, 1 PFlop/s

IBM Blue Gene/Q JUQUEEN 5.9 PFlop/s

IBM Blue Gene/Q JUQUEEN successor ~ 50 PFlop/s

Highly Scalable System
The Human Brain Project

Future & Emerging Technologies flagship project (co-)funded by European Commission

- Science-driven, seeded from FET, extending beyond ICT
- Ambitious, unifying goal, large-scale

Goal

- To build an integrated ICT infrastructure enabling a global collaborative effort towards understanding the human brain, and ultimately to emulate its computational capabilities

HBP sub-projects include:

- Strategic Human Brain Data (Amunts, Jülich)
- The Brain Simulation Platform (Markram, EPFL)
- High Performance Analytics & Computing Platform (Lippert, Jülich)
Objective: High-resolution Brain Atlas

Research goal

- Accurate, highly detailed computer model of the human brain based on histological input

Approach

- Create high-resolution 2-dimensional brain section images
- Re-construct 3-dimensional models from these images

[K. Amunts et al., Science 2013]
Need for High Resolution

- Large-Area Polarimeter image
  - Optical resolution limit = 159 μm
  - ~3 GByte / image

- Polarizing Microscope image
  - Optical resolution limit = 3.9 μm
  - ~700 GByte / image

[Julia Reckfort et al., 2015]
Objective: Brain Simulation using NEST

Application target
- Create models of the brains of mammals and humans
- Push limits of large-scale simulations of biologically realistic networks
  - Huge network: $O(10^{11})$ neurons
  - High connectivity: Neuron connected to $O(10^4)$ neurons

Approach
- Simulation of spiking neuronal network
- Focus on large networks, use of simple point neurons

[Potjans, Diesmann, 2012]
High Performance Analytics and Computing Platform

Heterogeneous distributed system comprising multiple resources allowing for

- Running large-scale, data intensive, interactive brain simulations up to the size of a full human brain
- Managing the large amounts of data produced by simulations or by neuroscience experiments
- Concurrent management of workloads and work-flows, data processing and visualization
Compute Challenge Brain atlas

Image registration
- Based on mutual information metric
- Determination of joint histograms
- Runs fast on current generation of NVIDIA GPUs
  - Key feature: support of L2 atomics

Navigation in petabytes of data
- About $O(10^{10}..100)$ GByte/image, $O(10^4)$ images
Data Transport: NVLink

Memory technology challenge

- Need for high-bandwidth $\triangleright$ GDDR5 or HBM
  - $O(10) \text{ GByte} @ O(100…1000) \text{ GByte/s}$
- Large capacity $\triangleright$ DDR3 or DDR4
  - $O(100) \text{ GByte} @ O(10…100) \text{ GByte/s}$

Opportunities created by NVLink

- Fast and fine-grained data transport host $\leftrightarrow$ device
- Multi-GPU nodes with larger aggregate memory
Compute Challenge Brain Simulator NEST

Simulation work-flow

- Construct network
- Spiking neuronal network simulations
- Analyze observables created by simulations

Supercomputer requirements

- Maximize memory footprint
  - Application today is memory capacity limited
- Optimize processing performance (concerns memory bandwidth)
  - Keep ratio simulation versus simulated time small
- Allow for interactive steering of the applications

[Kunkel et al., 2014]
Interactive Supercomputing Use Cases

Monitoring simulations
- Network may develop pathological behaviour
- Interactive access would allow for timely abortion

Interactive data selection
- Expensive data recording → must select recorded data
- Idea: Re-run simulation after first analysis

[M. Diesmann, 2013]
Use Cases (cont.)

Virtual surgery

- Scientific question: What happens if particular neuron connections are cut?
- Question can be addressed by interactive manipulation of network during simulation
  - Early results have already been published [Potjans, Diesmann, 2012]
Interactive Supercomputing Requirements

Integration of dense memory
- Increase memory footprint

Realise scalable visualisation capabilities
- Allow for inspection of data
- Involves in-situ data analysis and extraction

Dynamic management of resources
- Dynamic change of resources allocated to
  - Large scale simulation
  - Data analytics pipelines
  - Visualization
Pre-Commercial Procurement

Instrument for procurement of R&D services
- Competitive processed organised in multiple stages

Current status
- Final phase started in July 2015
- Remaining competitors
  - CRAY
  - IBM + NVIDIA
- Expect pilot systems to demonstrate readiness of technology in summer 2016
Conclusions

The Human Brain Project will facilitate exciting science

- High-resolution anatomic models of the brain
- Simulations based on models of realistic complexity

Applications from the Human Brain Project help to drive development of future supercomputers

- Need for exascale compute capabilities
- Extreme scale data challenges
- Use cases for interactive supercomputing