High Performance Computing for Weather and Climate (HPC4WC)

Content: Distributed Memory Parallelism / MPI
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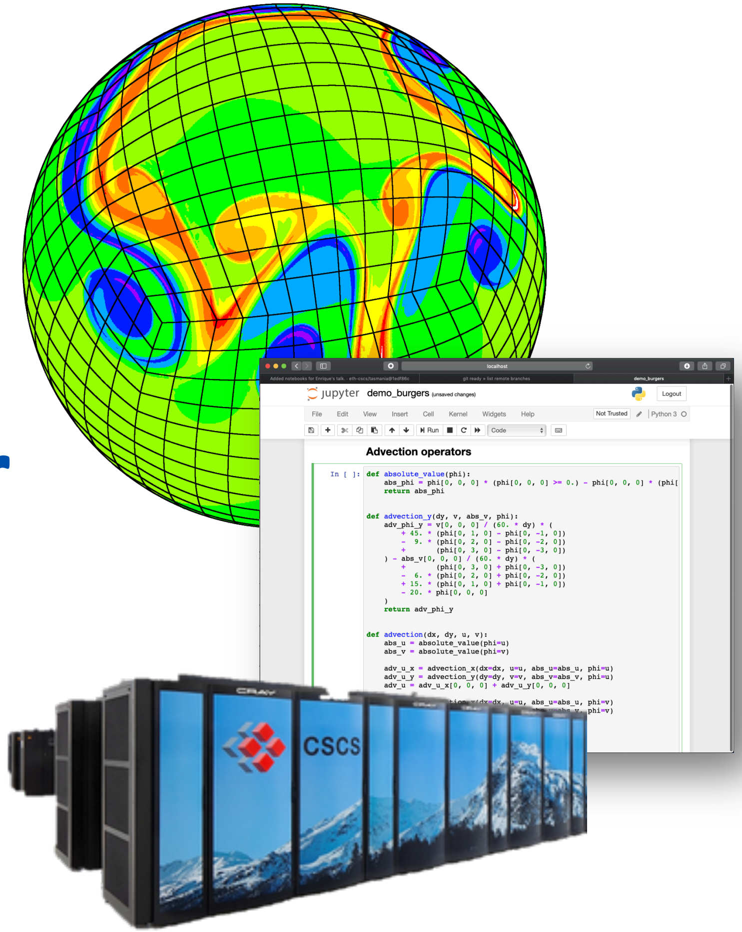
Block course 701-1270-00L
Summer 2020

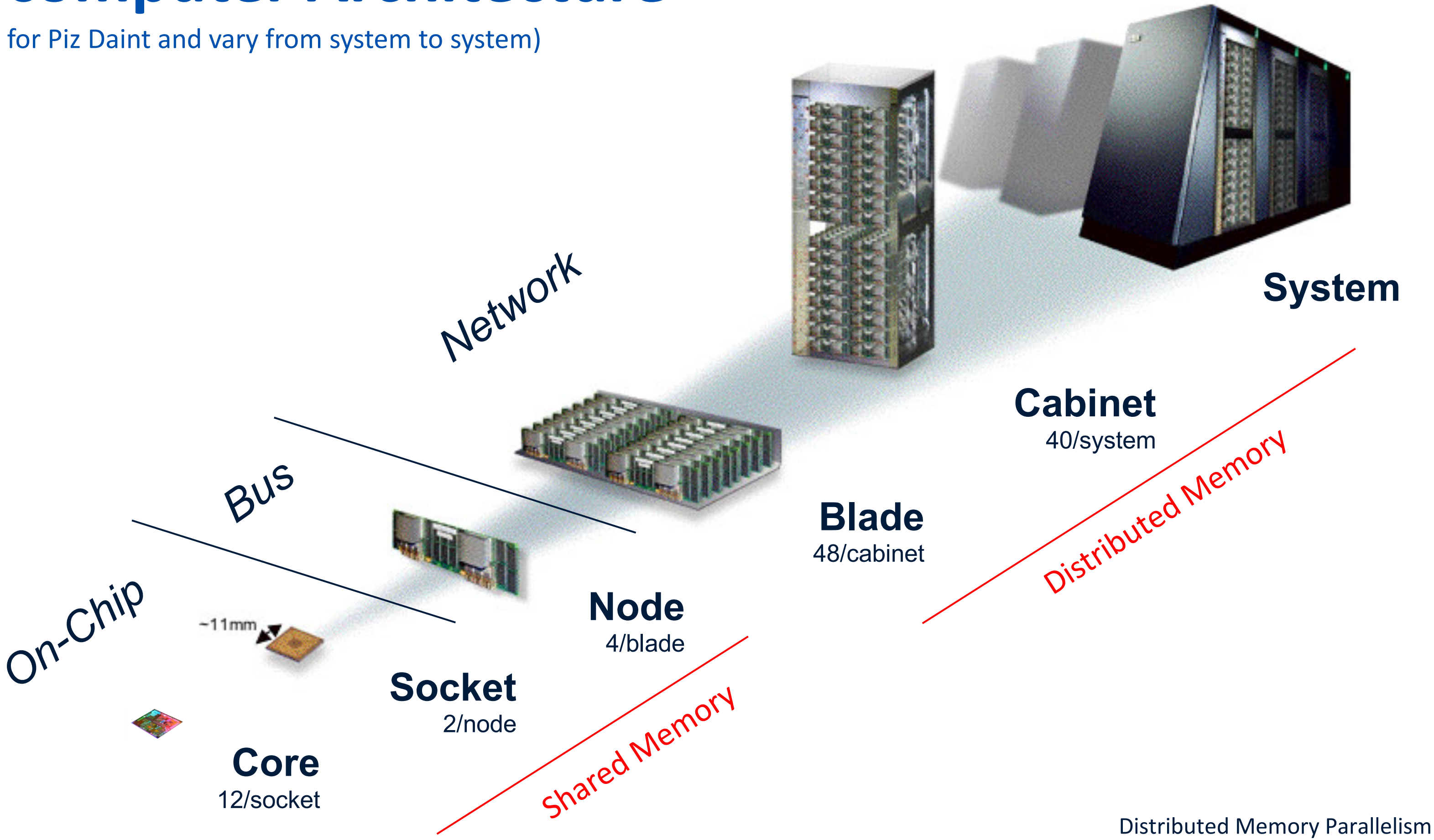


Learning goals

- Understand distributed memory parallelism and how it is different from shared memory parallelism
- Learn basic message passing patterns using MPI
- Be able to apply domain decomposition for solving partial differential equations
- Understand the concept of halo points and able to implement a halo-update.

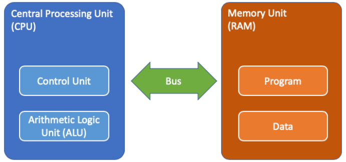
Supercomputer Architecture

(Numbers are for Piz Daint and vary from system to system)

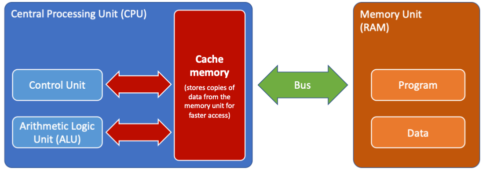


Computer Architecture

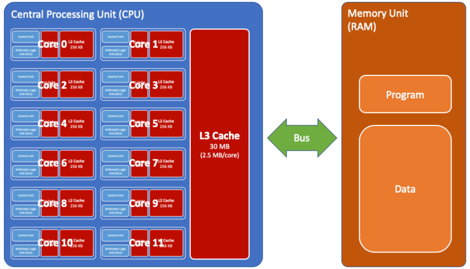
Von Neumann



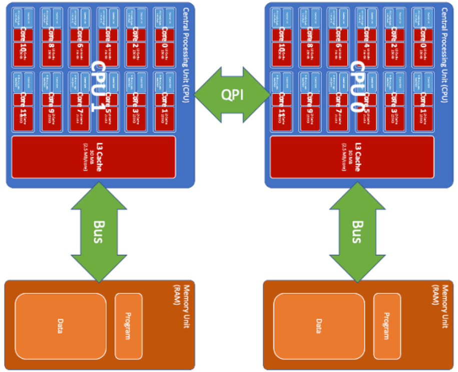
Cache hierarchy



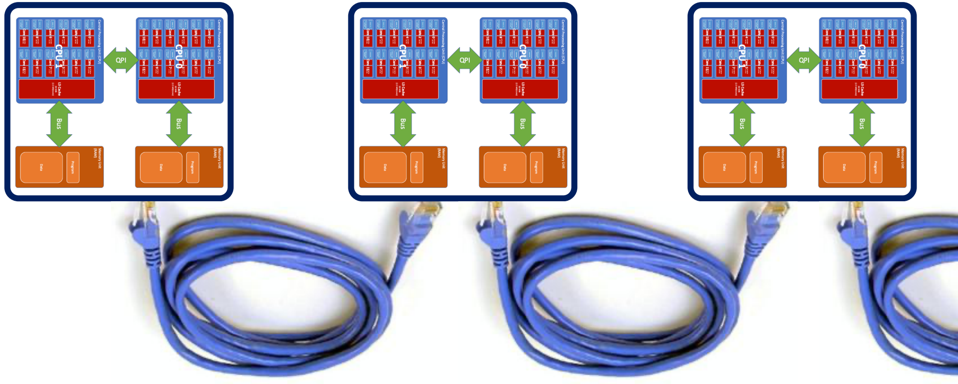
Modern CPU



Multicore Node



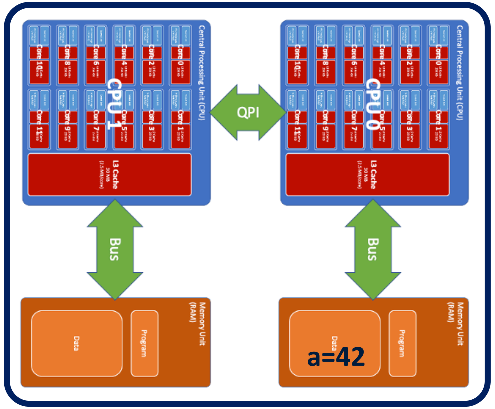
Many nodes



Distributed Memory

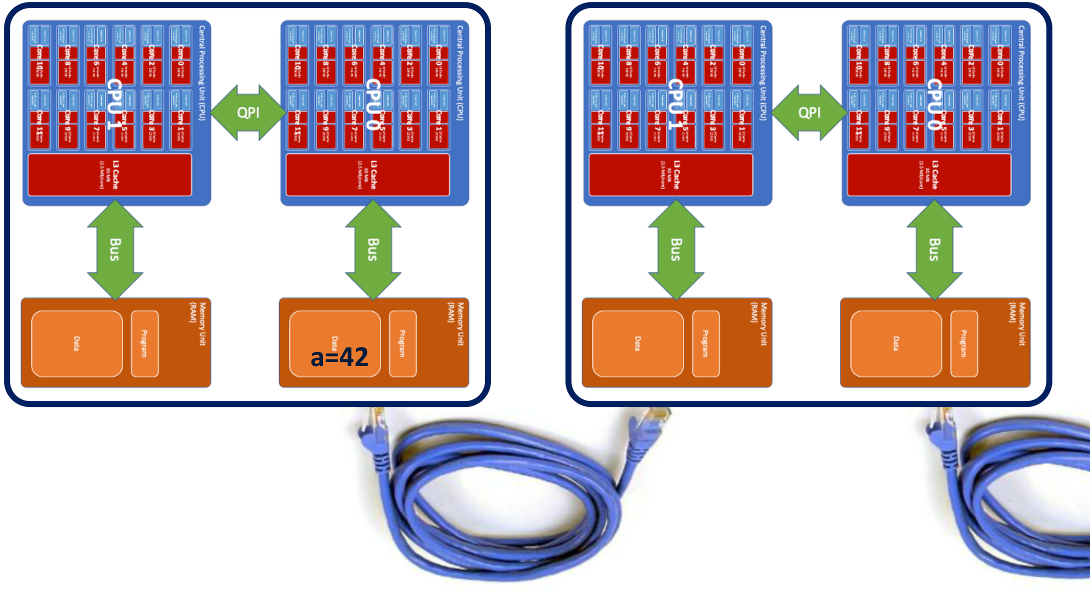
All cores on a node share the same address space / memory

```
>>> print(a)
42
```



Nodes have different address spaces / memories.
Variables are not shared.

```
>>> print(a)
NameError: name 'a' is not defined
```

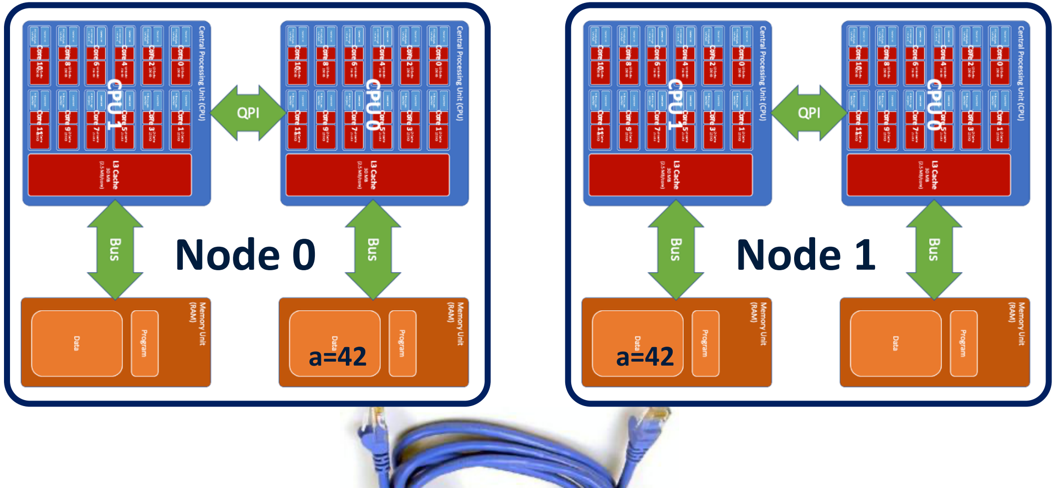


Message Passing

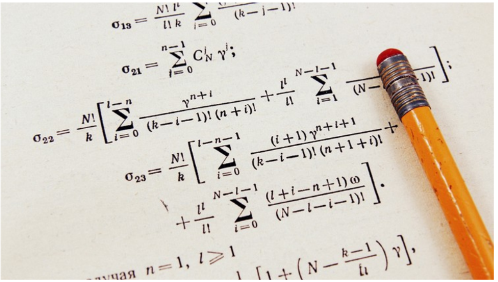
- Information between nodes is transferred over a network cable using a message passing protocol.

```
>>> send(a, destination=1)
>>> address(a)
0x001a947e3211
```

```
>>> a = recv(source=0)
>>> print(a)
42
>>> addres(a)
0x002f33498e77
```



Parallel Computing



Message Passing Interface (MPI)

- MPI is a standardized and portable message passing standard. (https://www.mpi-forum.org/ and https://github.com/mpi-forum)
- Version 1.0 in 1992, latest Version 3.1 in 2015, Version 4.0 ratification in progress
- Support for Fortran, C, C++, Python, Julia, …
- Implemented as a library that provides message passing semantics.
- Several implementations
  - MVAPICH
  - OpenMPI
  - Cray MPI
  - …
- Available on almost any architecture
  - Linux Laptop (apt-get install mpich)
  - Supercomputer
  - Google Cloud Platform
  - …

Lab Exercises

01-test-MPI-setup.ipynb

- Test the setup of your JupyterHub Server to make sure that MPI is working correctly.

02-MPI-introduction.ipynb

- Step-by-step introduction to MPI concepts in Python (mpi4py).

03-domain-decomposition.ipynb

- Learn about domain-decomposition.
- Apply domain-decomposition to a simple 1d example.
- Apply domain-decomposition to the stencil2d.py program.