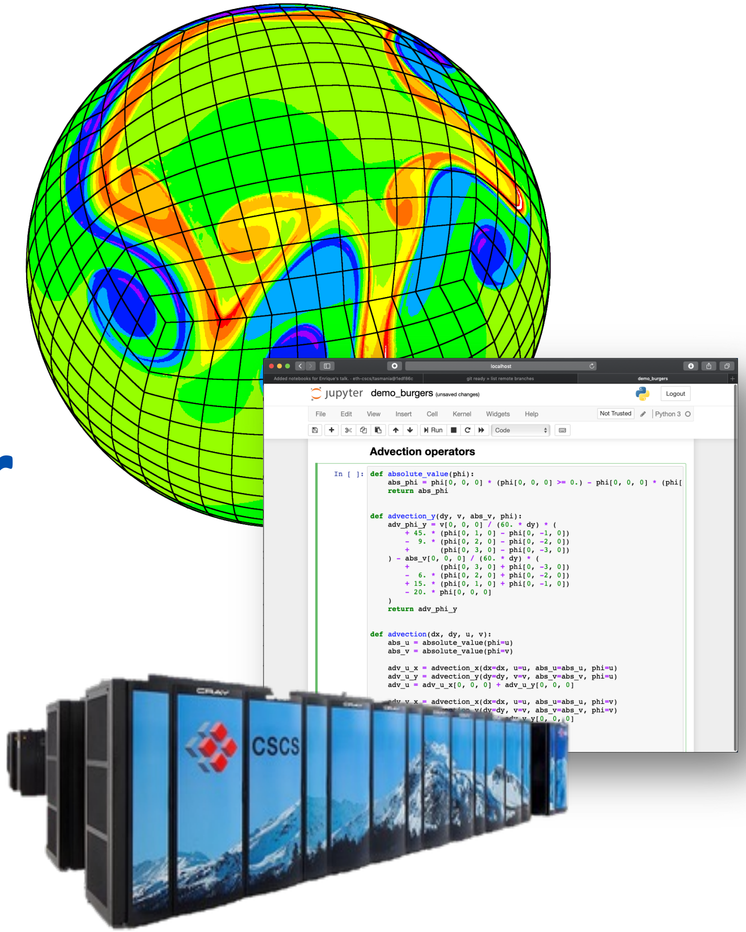
High Performance Computing for Weather and Climate (HPC4WC)



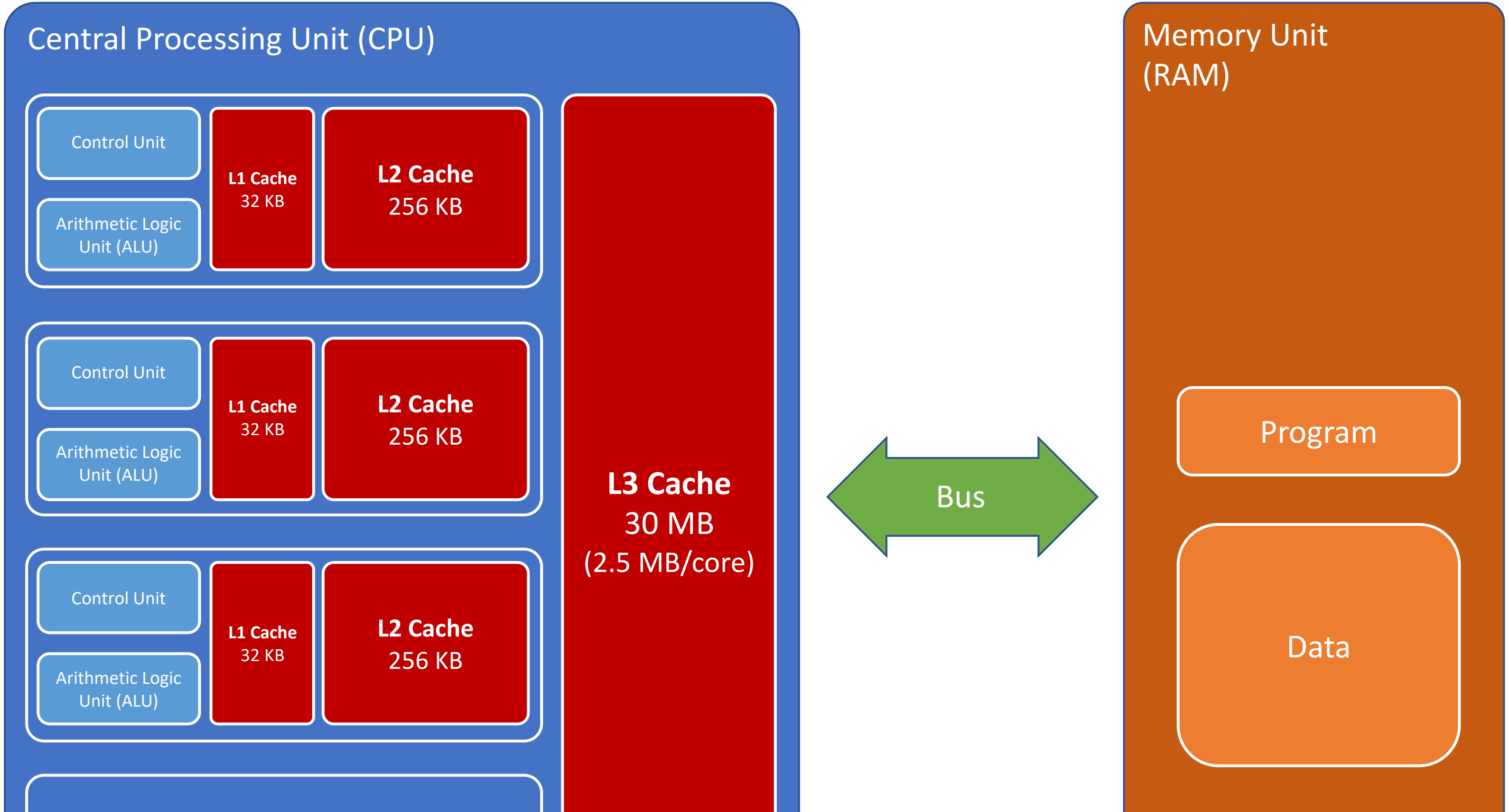
Content: Distributed Memory Parallelism / MPI
Lecturers: Oliver Fuhrer
Block course 701-1270-00L
Summer 2024

What speedup would you expect on 12 cores for a large, trivially parallel work task if it is compute bound?

(baseline: same code on 1 core)

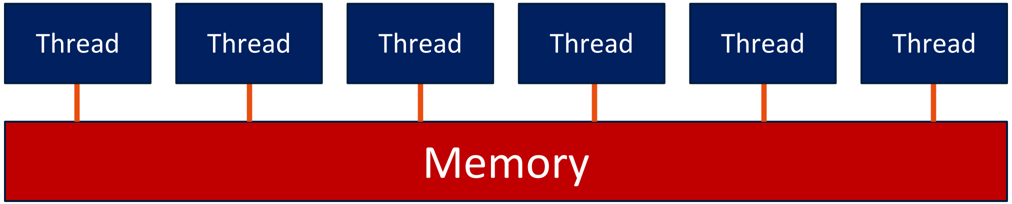
What if it is memory bandwidth bound?

Memory hierarchy (L1, L2, L3, DRAM)

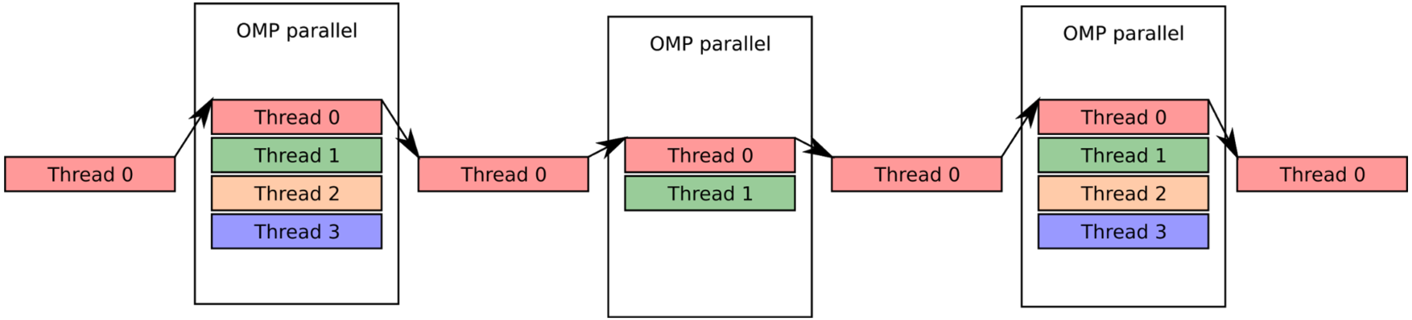


Shared memory parallelism

Parallel workers (threads) share the same view of memory



Fork-join model (threads)



OpenMP directives

For weather and climate models, most of the work is in loops over all gridpoints

```
!$omp parallel do default(none) private(tmp1_field, laplap) &
!$omp shared(nz, num_halo, ny, nx, in_field, num_iter, out_field, alpha)
do k = 1, nz
    do j = 1 + num_halo - 1, ny + num_halo + 1
    do i = 1 + num_halo - 1, nx + num_halo + 1
        tmp1_field(i, j) = -4._wp * in_field(i, j, k)        &
            + in_field(i - 1, j, k) + in_field(i + 1, j, k)  &
            + in_field(i, j - 1, k) + in_field(i, j + 1, k)
    end do
```

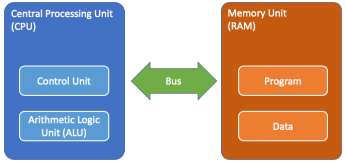
Step 0: Determine where most of the time is spent (e.g. using a profiler)
Step 1: Determine what can be run in parallel, apply OpenMP directives
Step 2: Apply data-sharing rules (e.g. specify which variables are private/shared)
Step 3: Optimize using profiler (e.g. schedule)
Repeat!

Learning goals

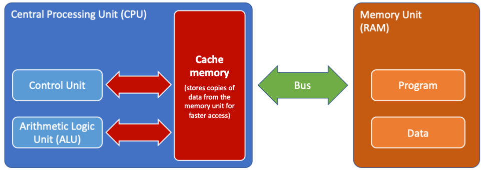
- Understand distributed memory parallelism and how it is different from shared memory parallelism
- Learn basic message passing patterns using MPI
- Be able to apply domain decomposition for solving partial differential equations
- Understand the concept of halo points and able to implement a halo-update.

Computer Architecture

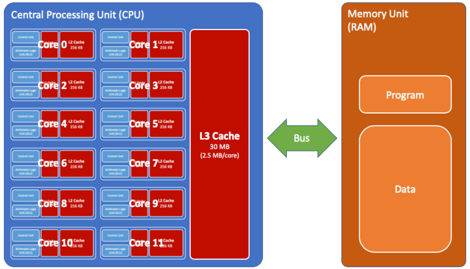
Von Neumann



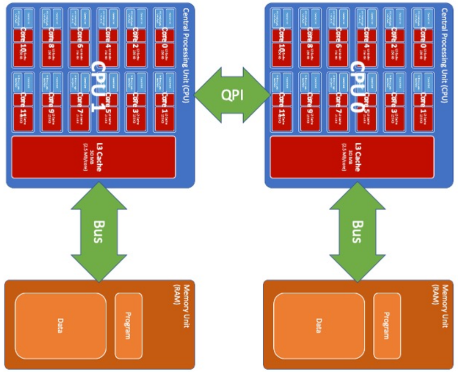
Cache hierarchy



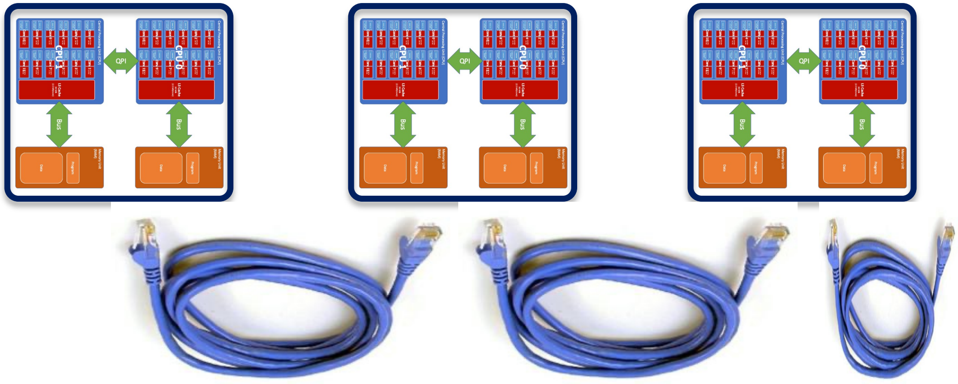
Modern CPU



Multicore Node



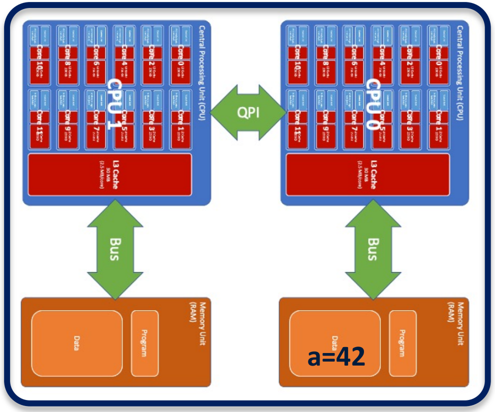
Many nodes



Shared vs. Distributed Memory

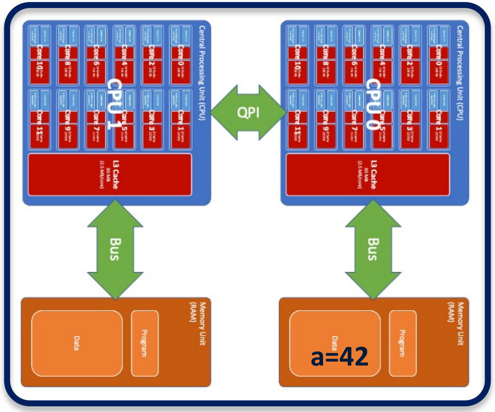
All cores on a node share the same address space / memory

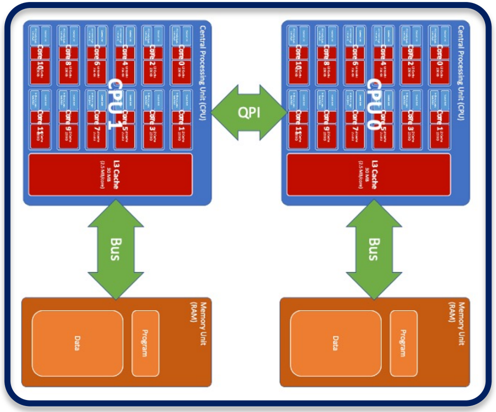
```
>>> print(a)
42
```



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

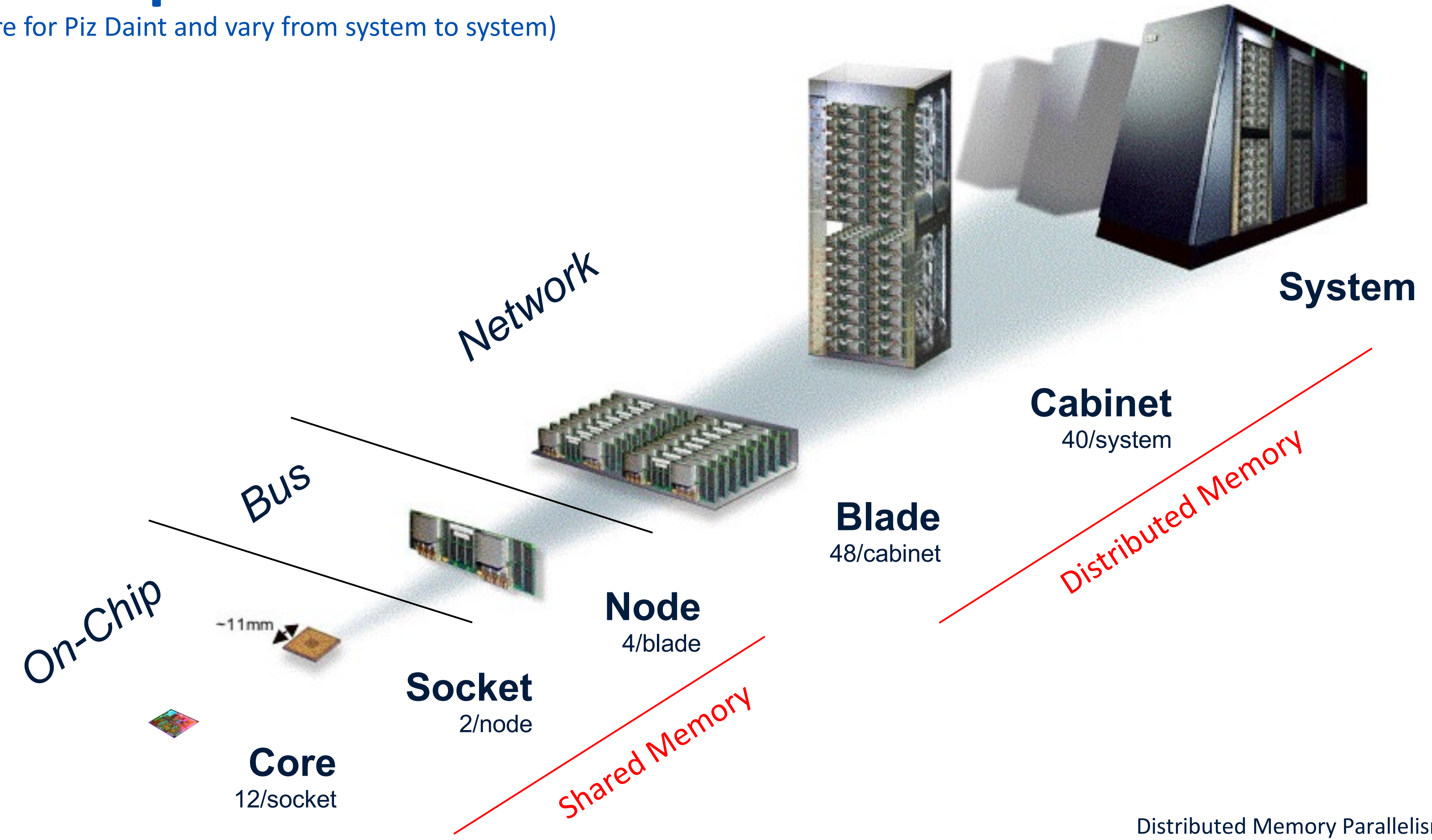
```
>>> print(a)
NameError: name 'a' is not defined
```





Supercomputer Architecture

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

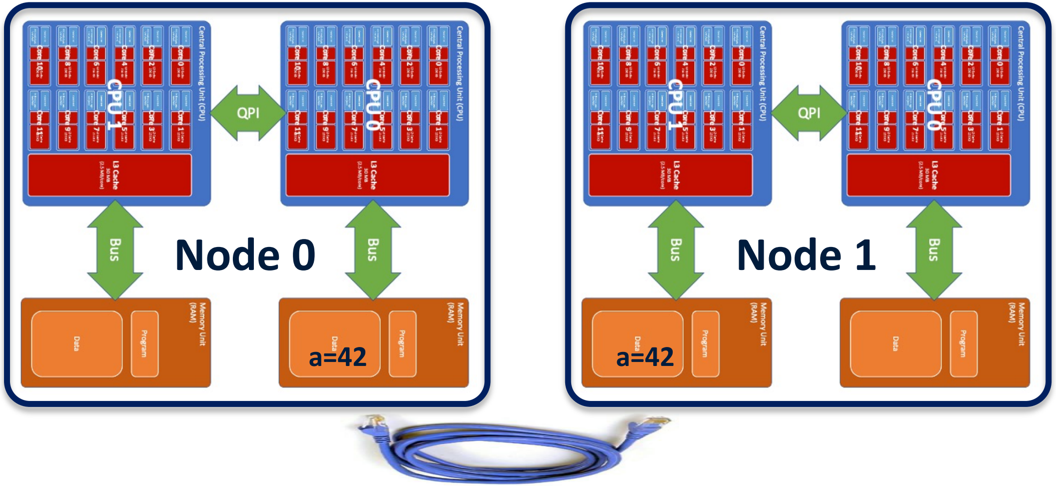


Message Passing

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

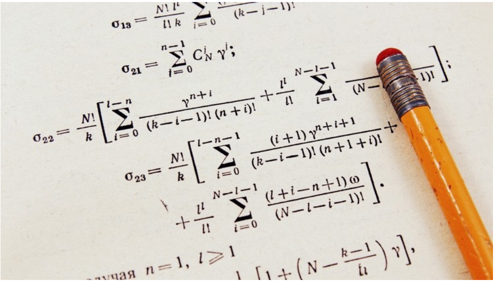
```
>>> a = 42
>>> address(a)
0x001a947e3211
>>> send(a, destination=1)
```

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



Parallel Computing (shared memory)

Problem



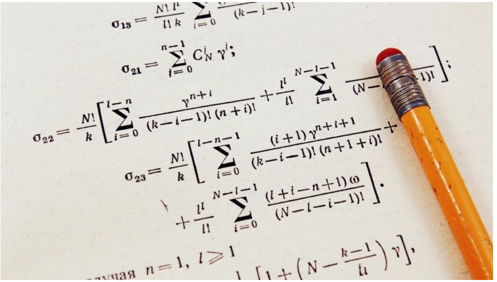
Worker 1

Worker 2

Notebook

Parallel Computing (distributed memory)

Problem



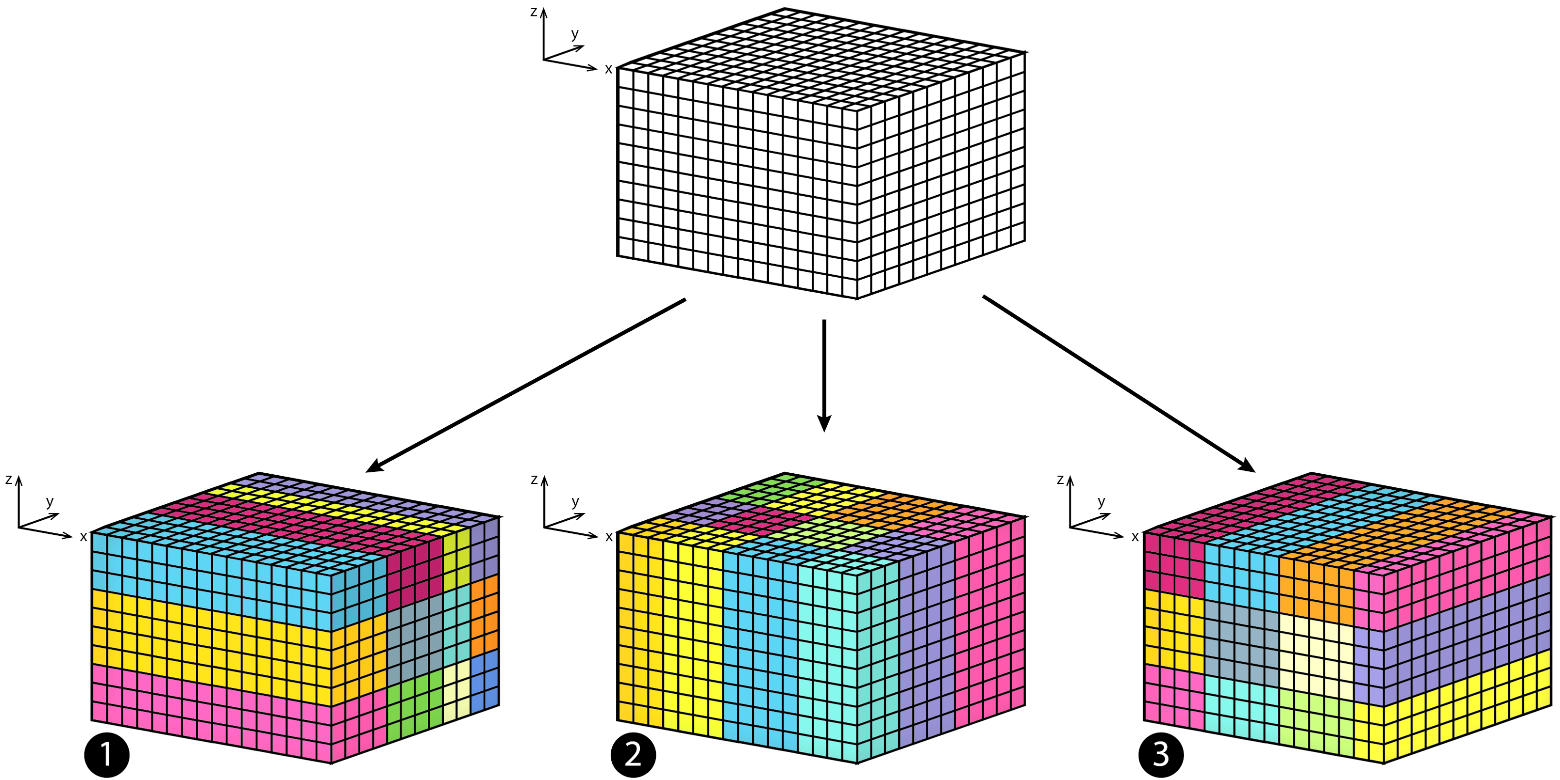
Worker 1

Worker 2

Notebook

Notebook

Domain Decomposition



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.

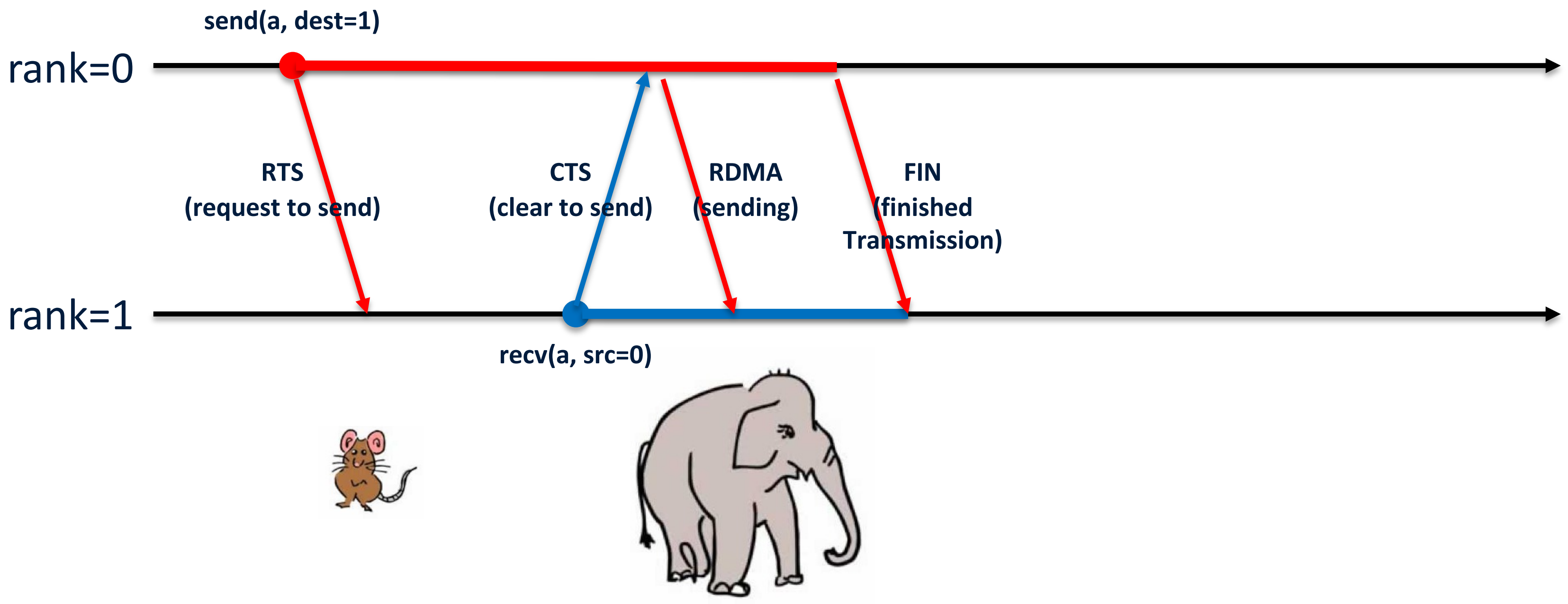
02-MPI-introduction.ipynb

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

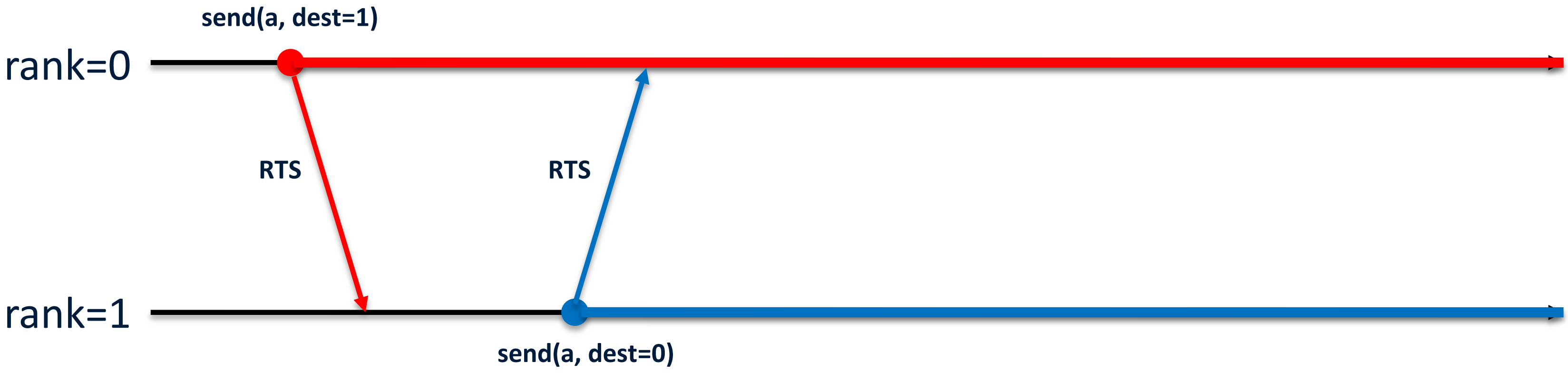
03-domain-decomposition.ipynb

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

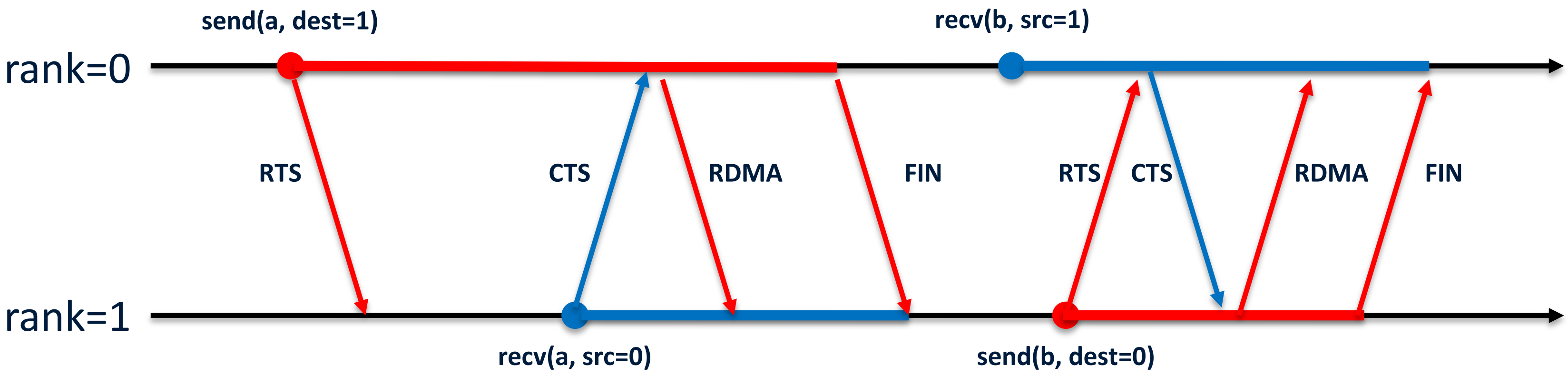
Send / Receive (Rendezvous protocol = large messages)



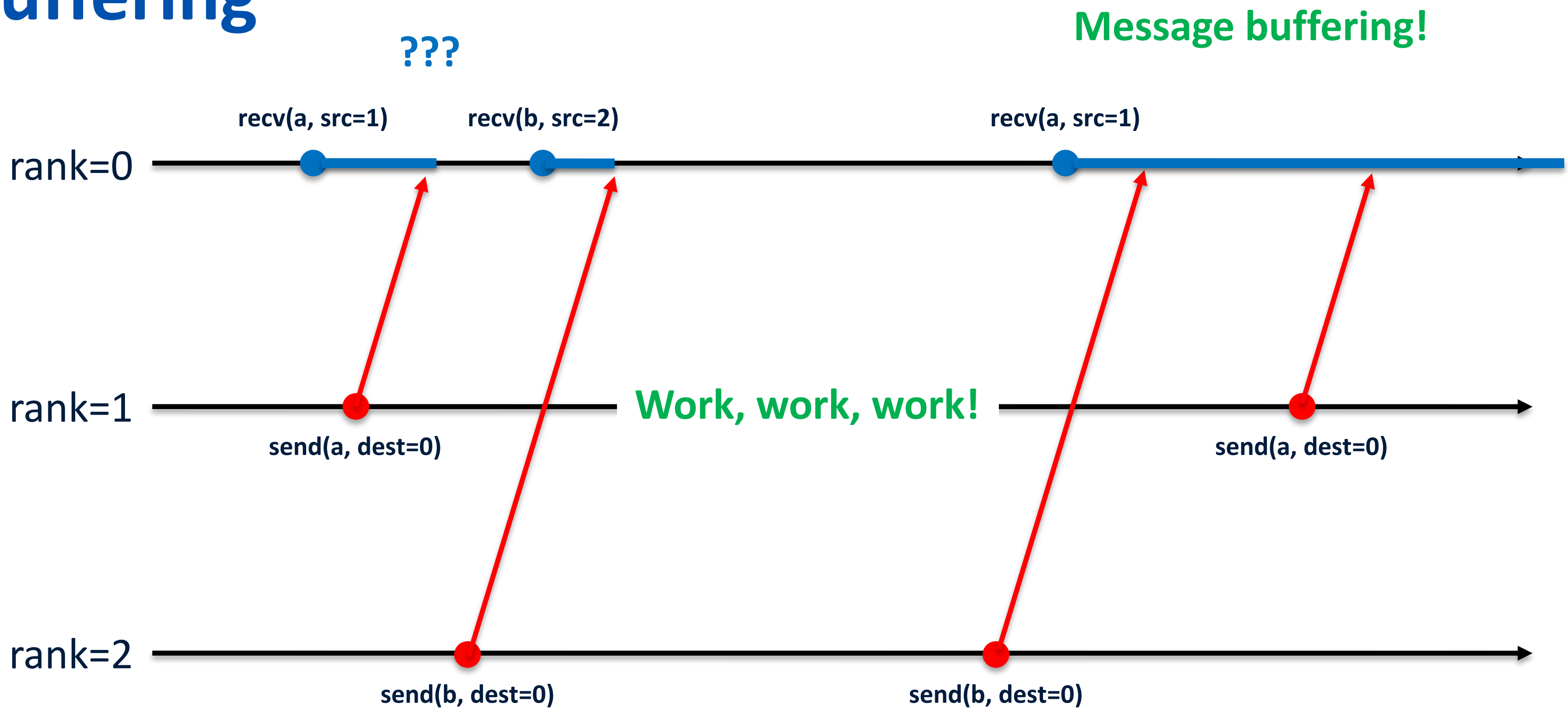
Deadlock



Matching Send / Recv

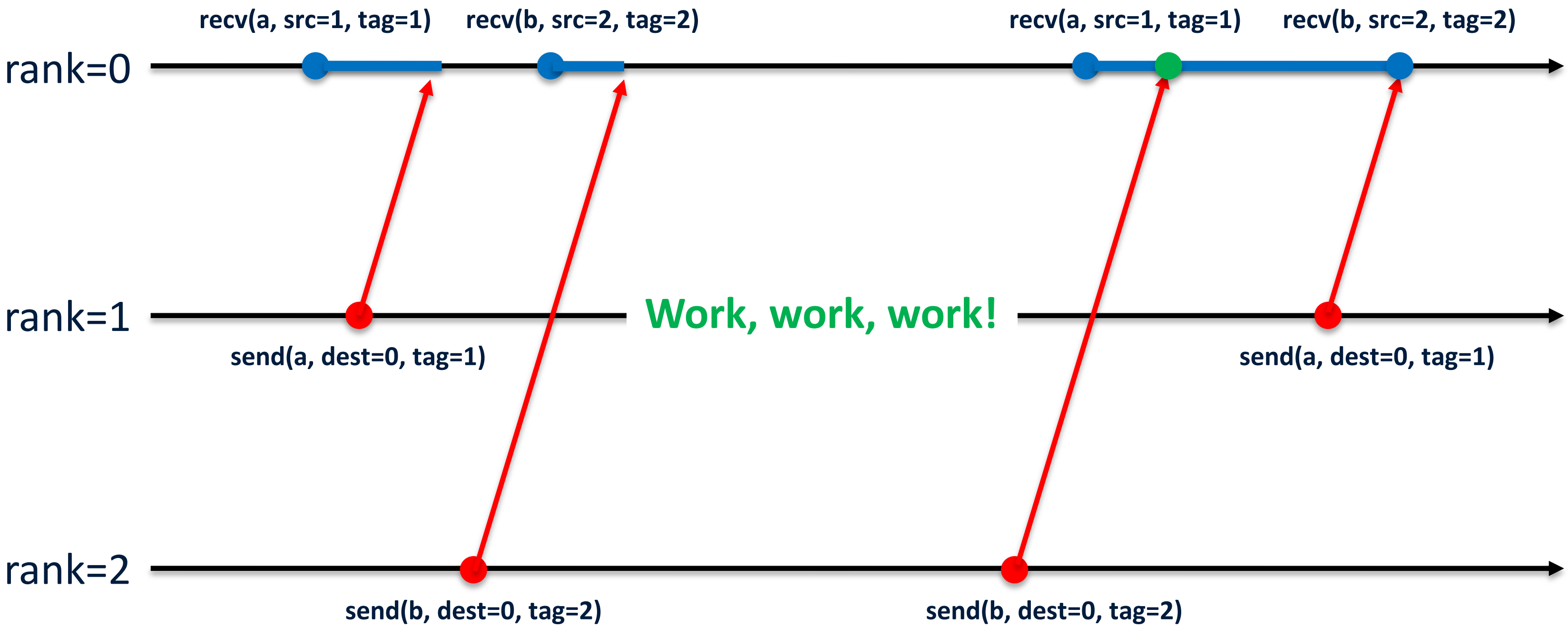


Buffering

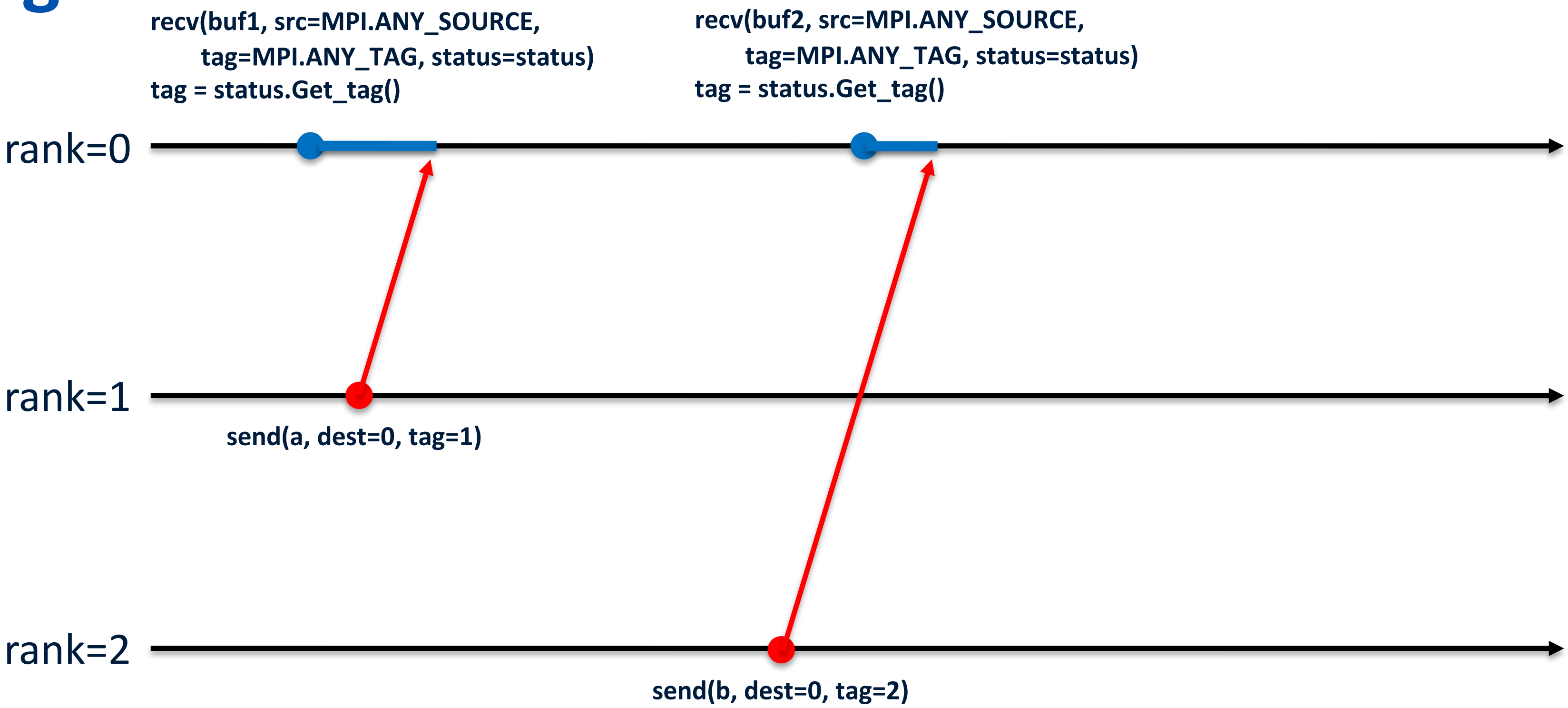


Message buffering!
???
recv(a, src=1)
recv(b, src=2)
recv(a, src=1)
rank=0
rank=1
Work, work, work!
send(a, dest=0)
send(a, dest=0)
rank=2
send(b, dest=0)
send(b, dest=0)

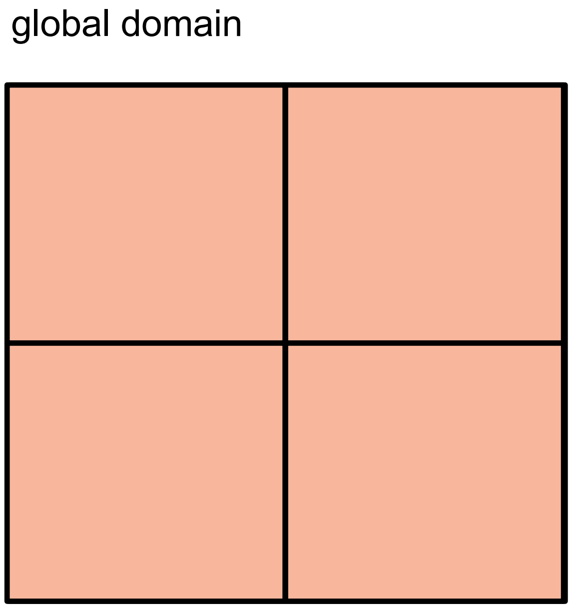
Tags

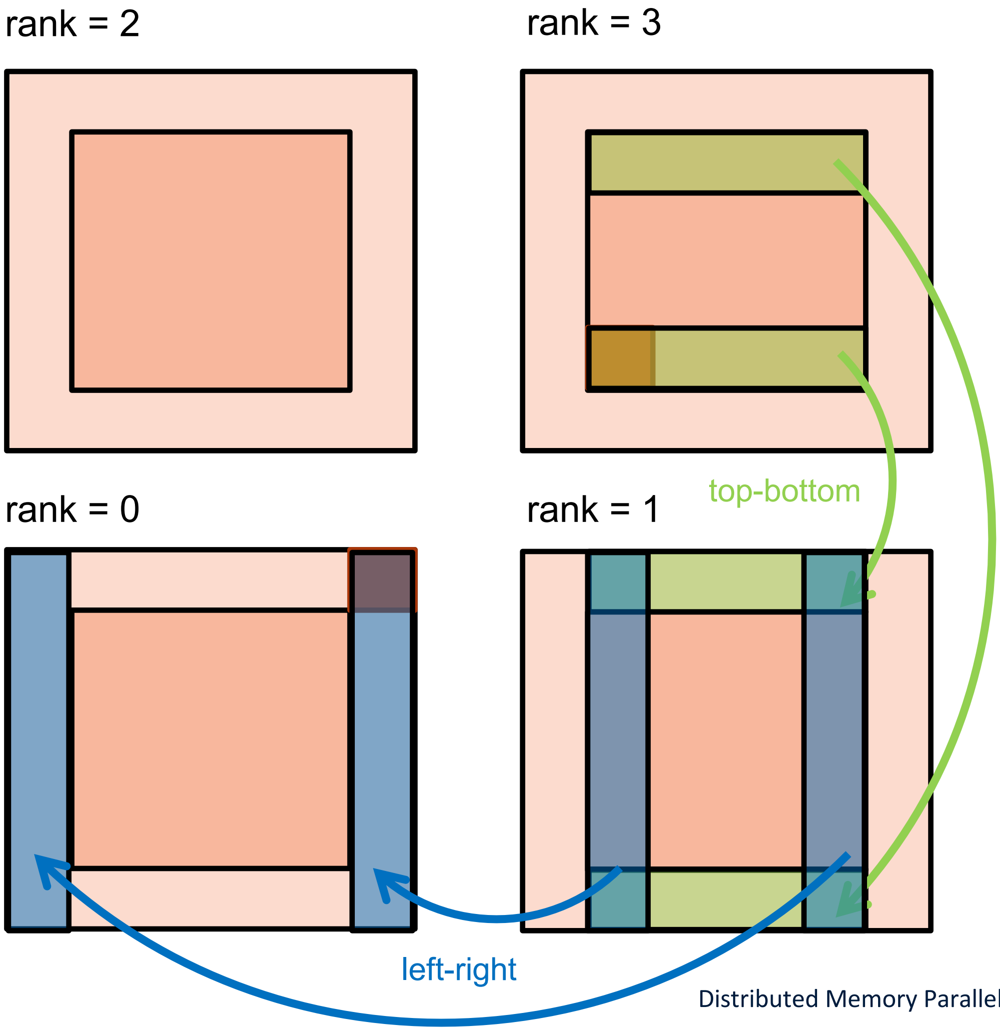

recv(a, src=1, tag=1)
recv(b, src=2, tag=2)
recv(a, src=1, tag=1)
recv(b, src=2, tag=2)
rank=0
rank=1
Work, work, work!
send(a, dest=0, tag=1)
send(a, dest=0, tag=1)
rank=2
send(b, dest=0, tag=2)
send(b, dest=0, tag=2)

Tags


recv(buf1, src=MPI.ANY_SOURCE,
tag=MPI.ANY_TAG, status=status)
tag = status.Get_tag()
recv(buf2, src=MPI.ANY_SOURCE,
tag=MPI.ANY_TAG, status=status)
tag = status.Get_tag()
rank=0
rank=1
send(a, dest=0, tag=1)
rank=2
send(b, dest=0, tag=2)

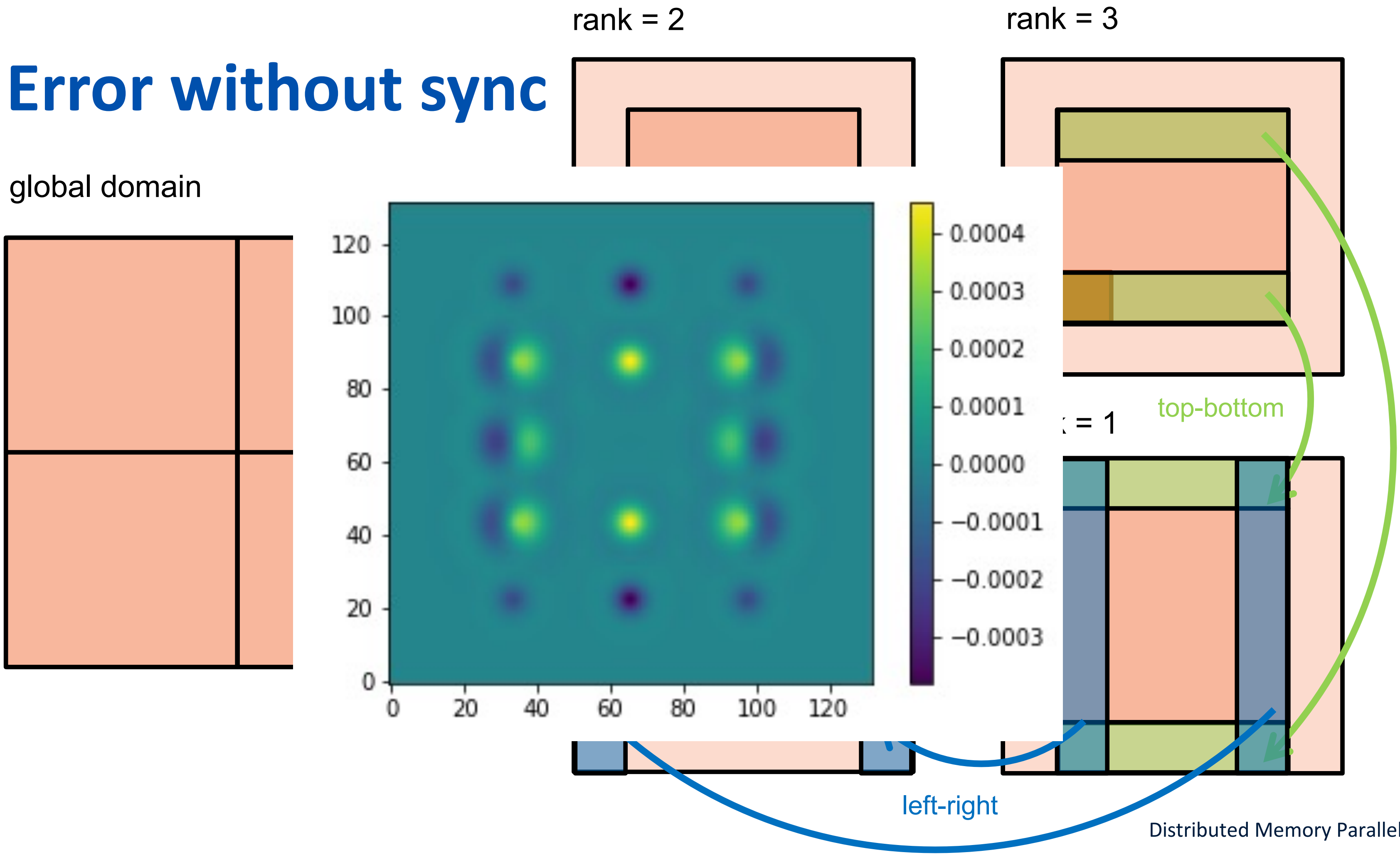
Corners


global domain


rank = 2
rank = 3
rank = 0
rank = 1
top-bottom
left-right

Error without sync

global domain



No-sync strategy

global domain