

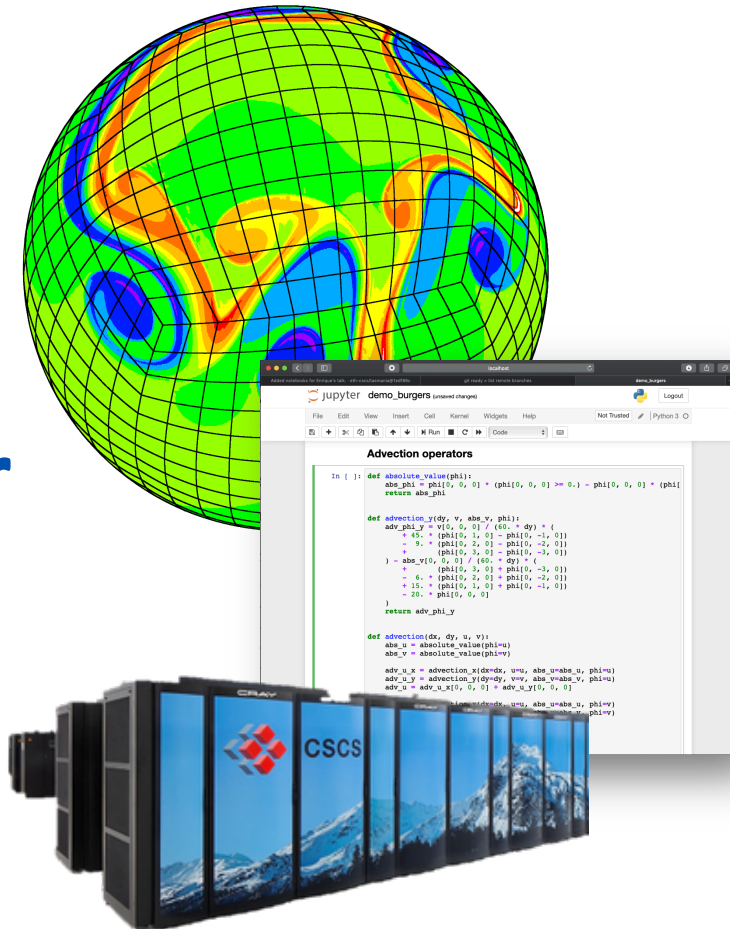
# High Performance Computing for Weather and Climate (HPC4WC)

Content: Distributed Memory Parallelism / MPI

Lecturers: Oliver Fuhrer

Block course 701-1270-00L

Summer 2020

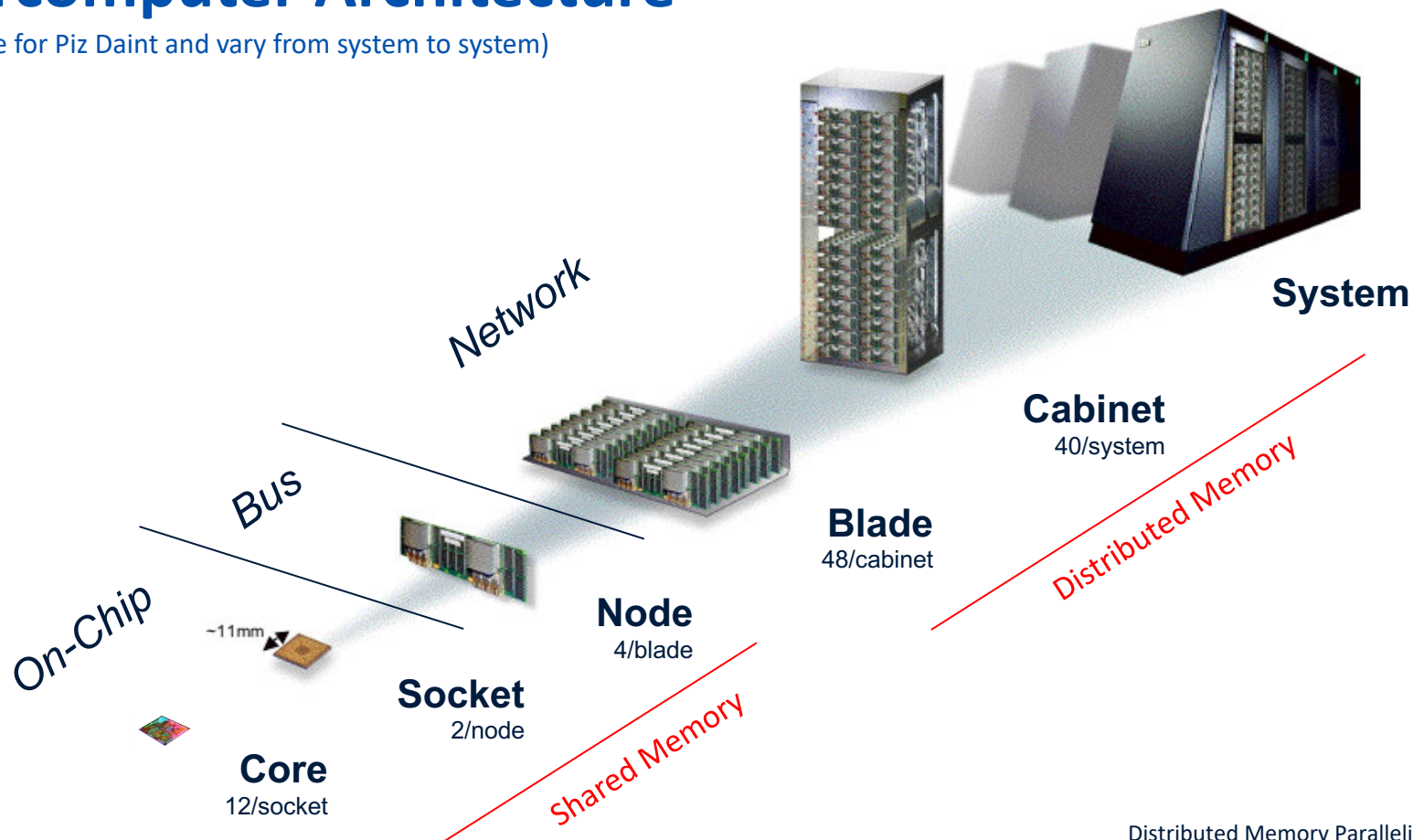


# Learning goals

- 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.

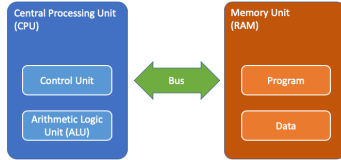
# Supercomputer Architecture

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

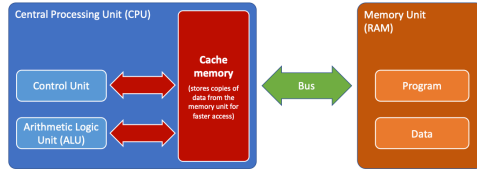


# Computer Architecture

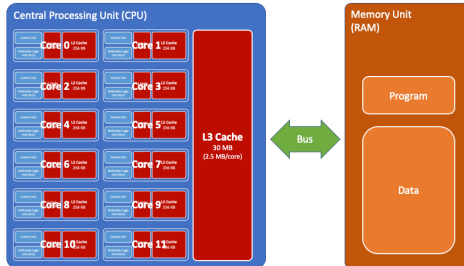
## Von Neumann



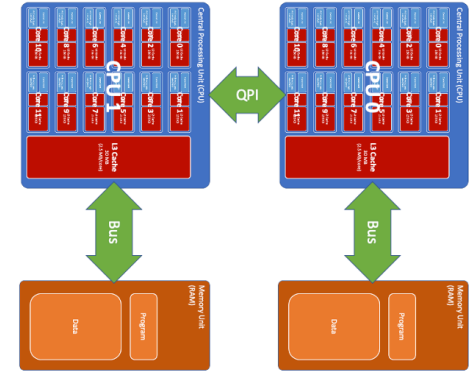
## Cache hierarchy



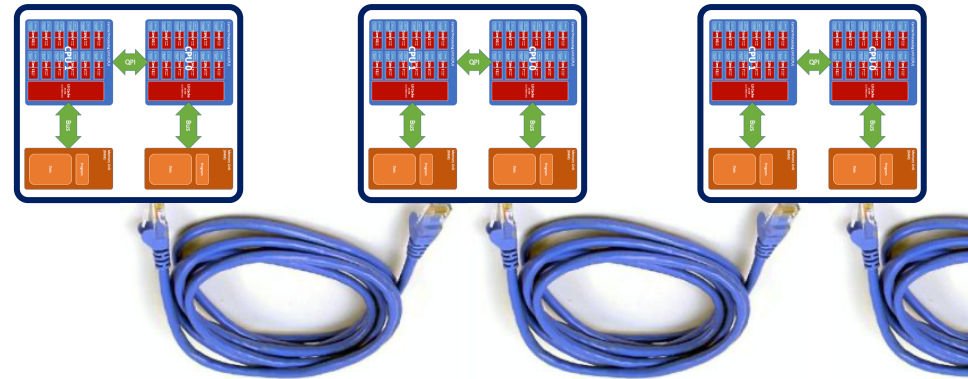
## Modern CPU



## Multicore Node



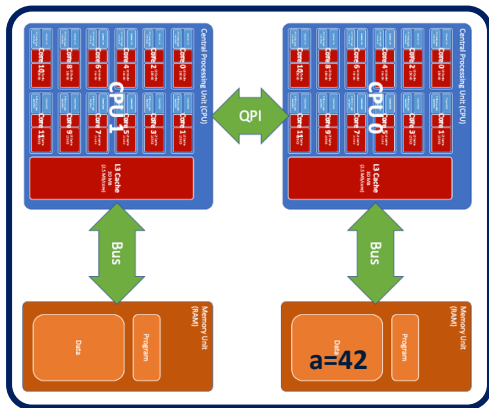
## Many nodes



# Distributed Memory

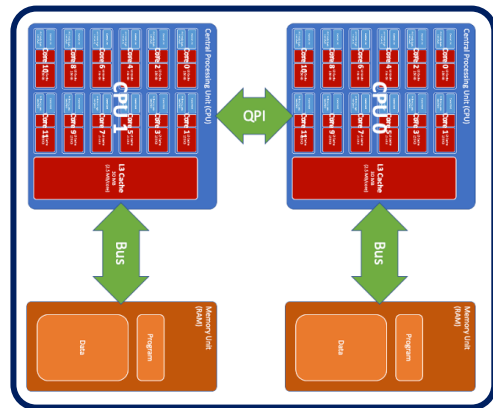
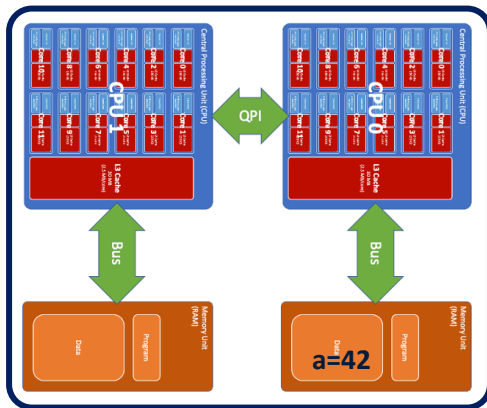
All cores on a node share the same address space / memory

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



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

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

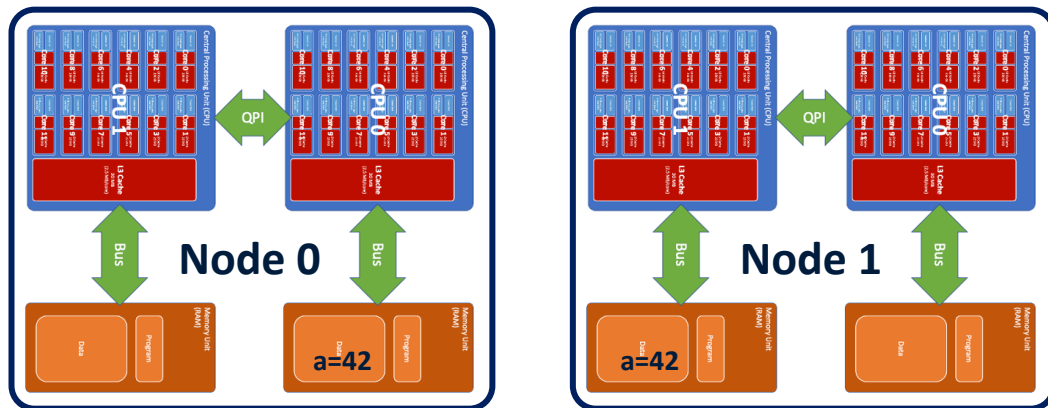


# Message Passing

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

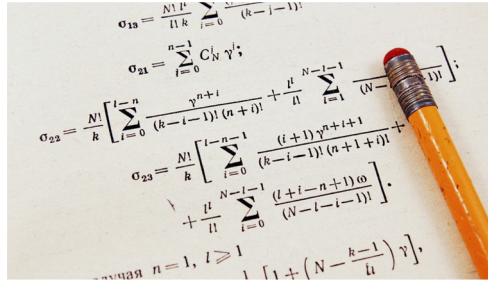
```
>>> send(a, destination=1)
>>> address(a)
0x001a947e3211
```

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



# Parallel Computing (shared memory)

Problem



Handwritten mathematical formulas on a piece of paper, with a yellow pencil resting on it. The formulas include:

$$\sigma_{10} = \frac{N!}{l!k} \sum_{i=0}^n \frac{\gamma_i}{(k-i-1)!}$$
$$\sigma_{21} = \sum_{i=0}^{n-1} C_N^i \gamma_i$$
$$\sigma_{22} = \frac{N!}{k} \left[ \sum_{i=0}^{l-n} \frac{\gamma^{n+i}}{(k-i-1)!(n+i)!} + \frac{l!}{l!} \sum_{i=1}^{N-l-1} \frac{1}{(N-i-1)!} \right]$$
$$\sigma_{23} = \frac{N!}{k} \left[ \sum_{i=0}^{l-n-1} \frac{(i+1)\gamma^{n+i+1}}{(k-i-1)!(n+i+1)!} + \frac{l!}{l!} \sum_{i=0}^{N-l-1} \frac{(l+i-n+1)\omega}{(N-l-i-1)!} \right]$$

Below the formulas, it says:  $n=1, l \geq 1$

Worker 1



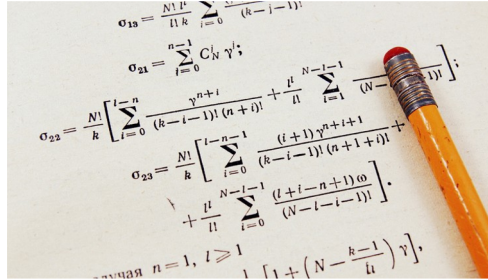
Worker 2



Notebook

# Parallel Computing (distributed memory)

Problem



Handwritten mathematical formulas on a piece of paper, with an orange pencil resting on it. The formulas include:

$$\sigma_{13} = \frac{N!}{l!k} \sum_{i=0}^{N-l-k} \frac{\gamma^{N-l-k-i}}{(k-i-1)!}$$
$$\sigma_{21} = \sum_{i=0}^{n-1} C_N^i \gamma^i$$
$$\sigma_{22} = \frac{N!}{k} \left[ \sum_{i=0}^{l-n} \frac{\gamma^{n+i}}{(k-i-1)! (n+i)!} + \frac{l!}{l!} \sum_{i=1}^{N-l-1} \frac{\gamma^{N-l-1-i}}{(N-i-1)!} \right]$$
$$\sigma_{23} = \frac{N!}{k} \left[ \sum_{i=0}^{l-n-1} \frac{(i+1) \gamma^{n+i+1}}{(k-i-1)! (n+i+1)!} + \frac{l!}{l!} \sum_{i=0}^{N-l-1} \frac{(l+i-n+1) \gamma}{(N-l-i-1)!} \right]$$

Below the formulas, it says:  $n=1, l \geq 1$

Worker 1



Notebook

Worker 2



Notebook

Distributed Memory Parallelism

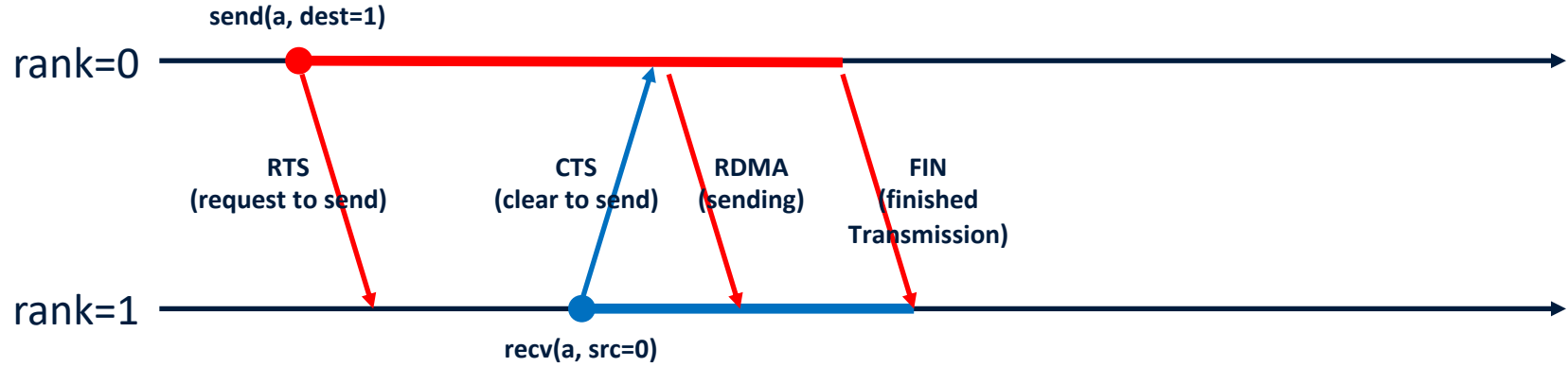


# Message Passing Interface (MPI)

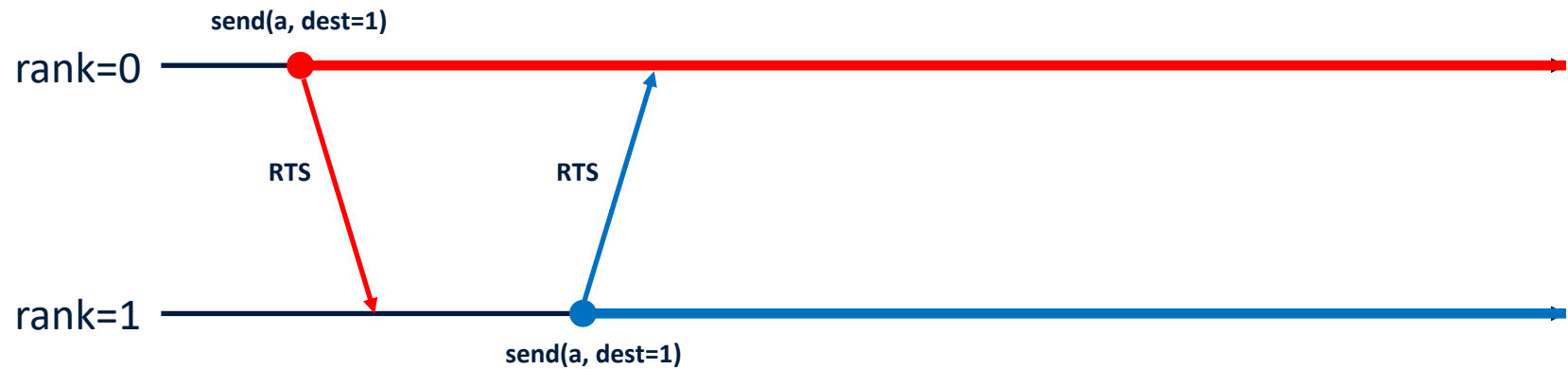


- MPI is a standardized and portable message passing standard.  
(<https://www.mpi-forum.org/> and <https://github.com/mpi-forum>)
- Version 1.0 in 1992, latest Version 3.1 in 2015, Version 4.0 ratification in progress
- Support for Fortran, C, C++, Python, Julia, ...
- Implemented as a library that 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
  - ...

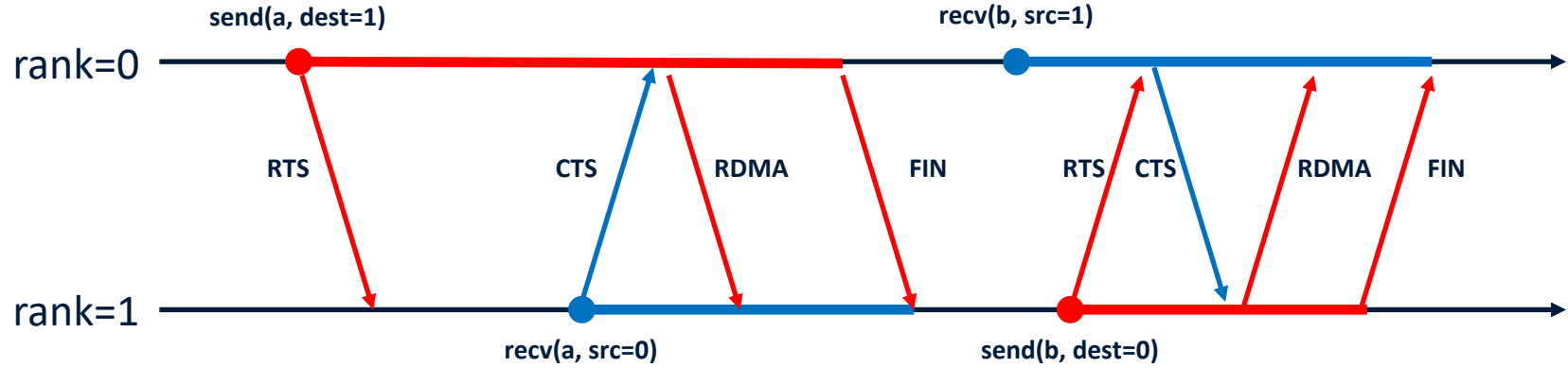
# Send / Receive



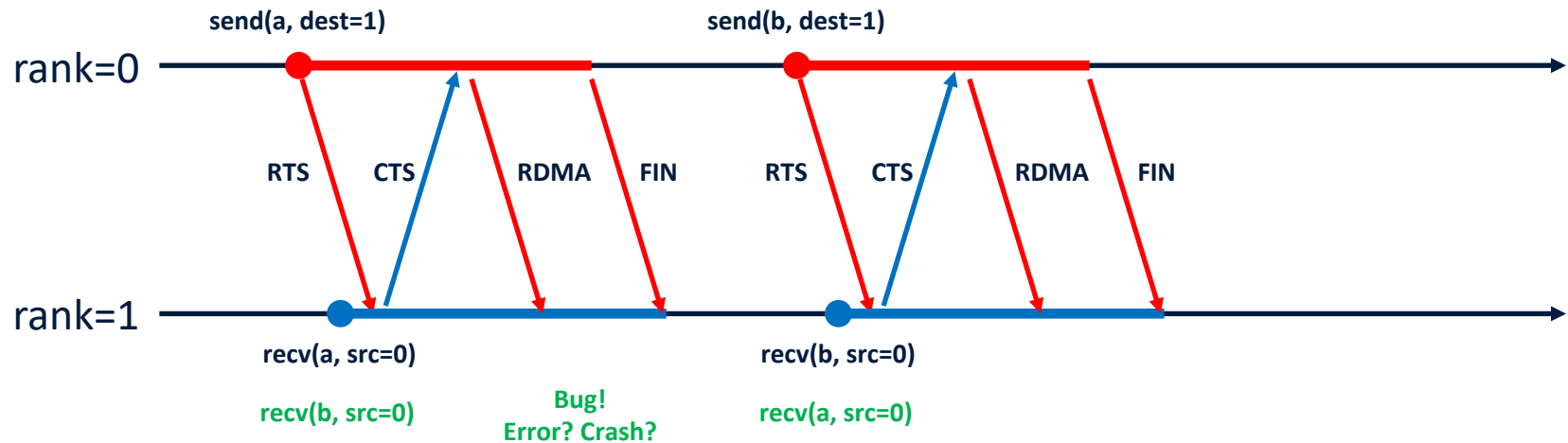
# Deadlock



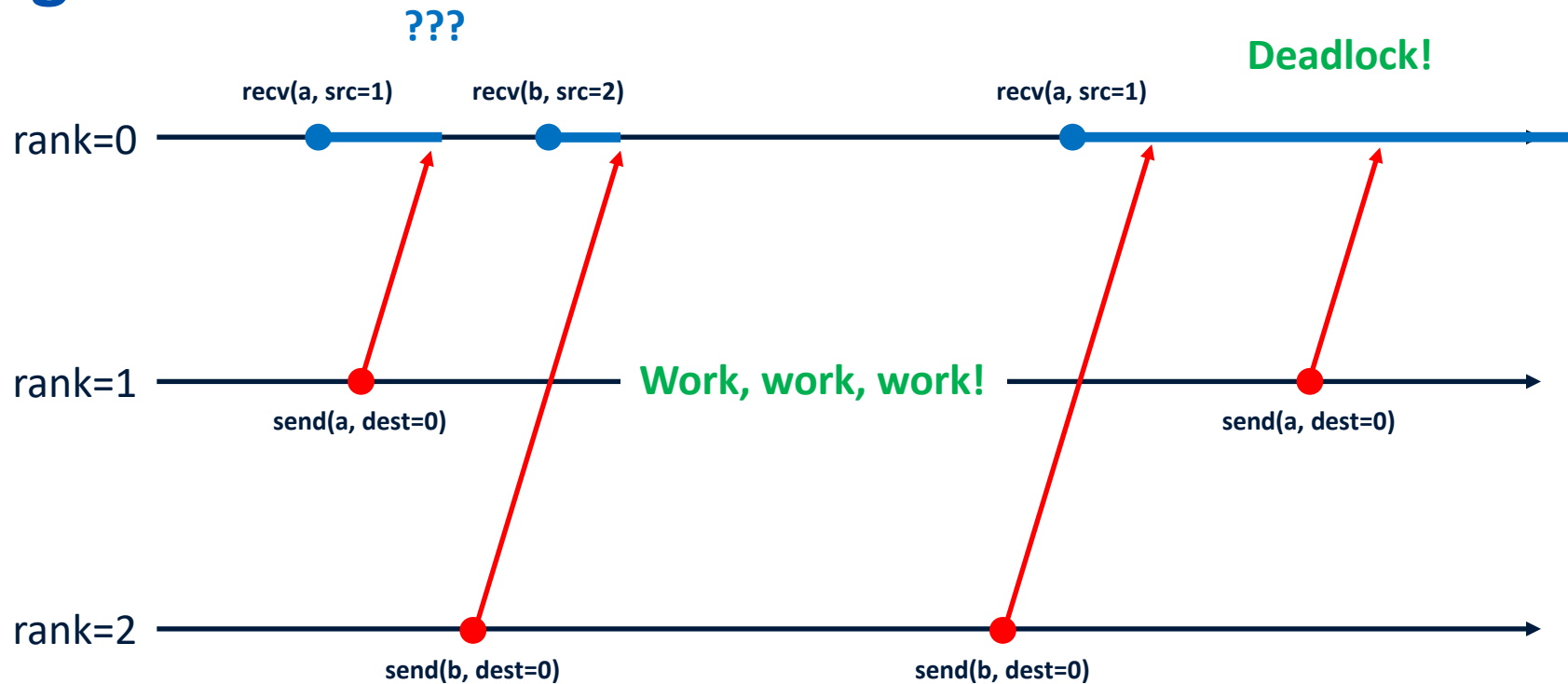
# Matching Send / Recv



# Message Order

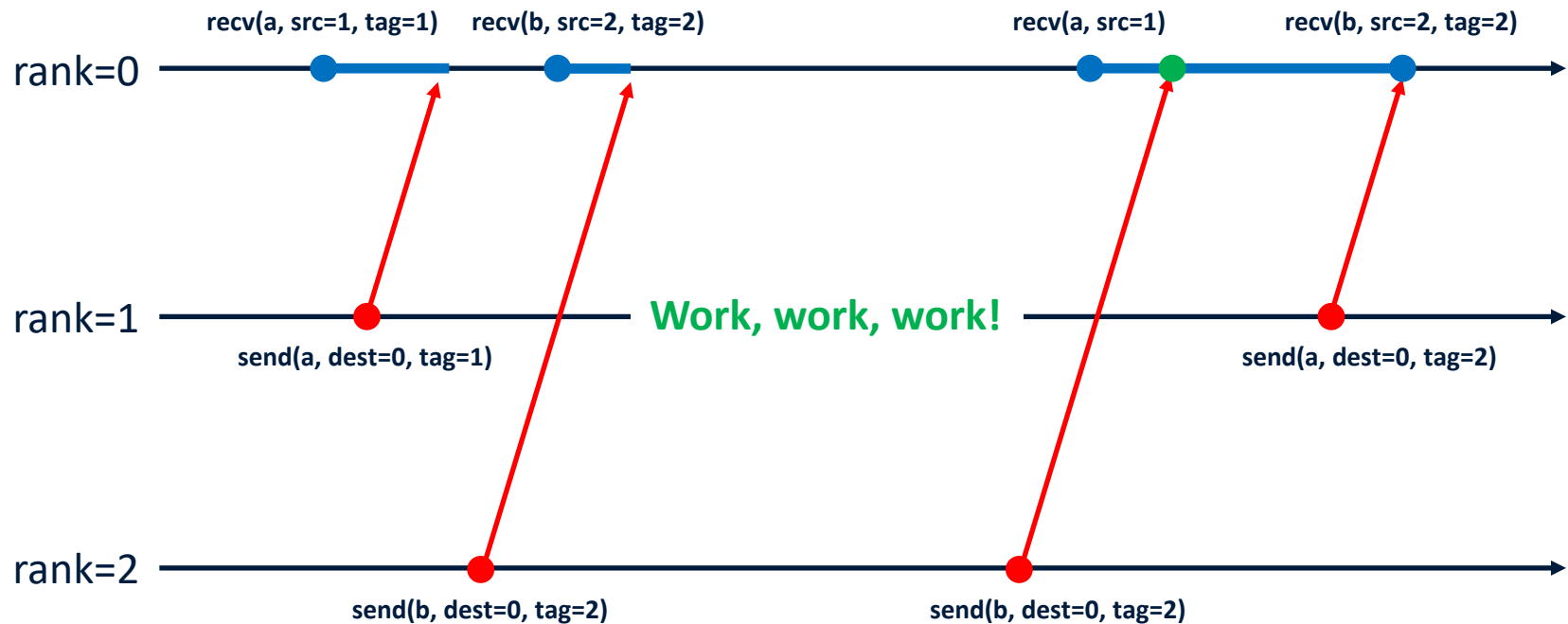


# Tags

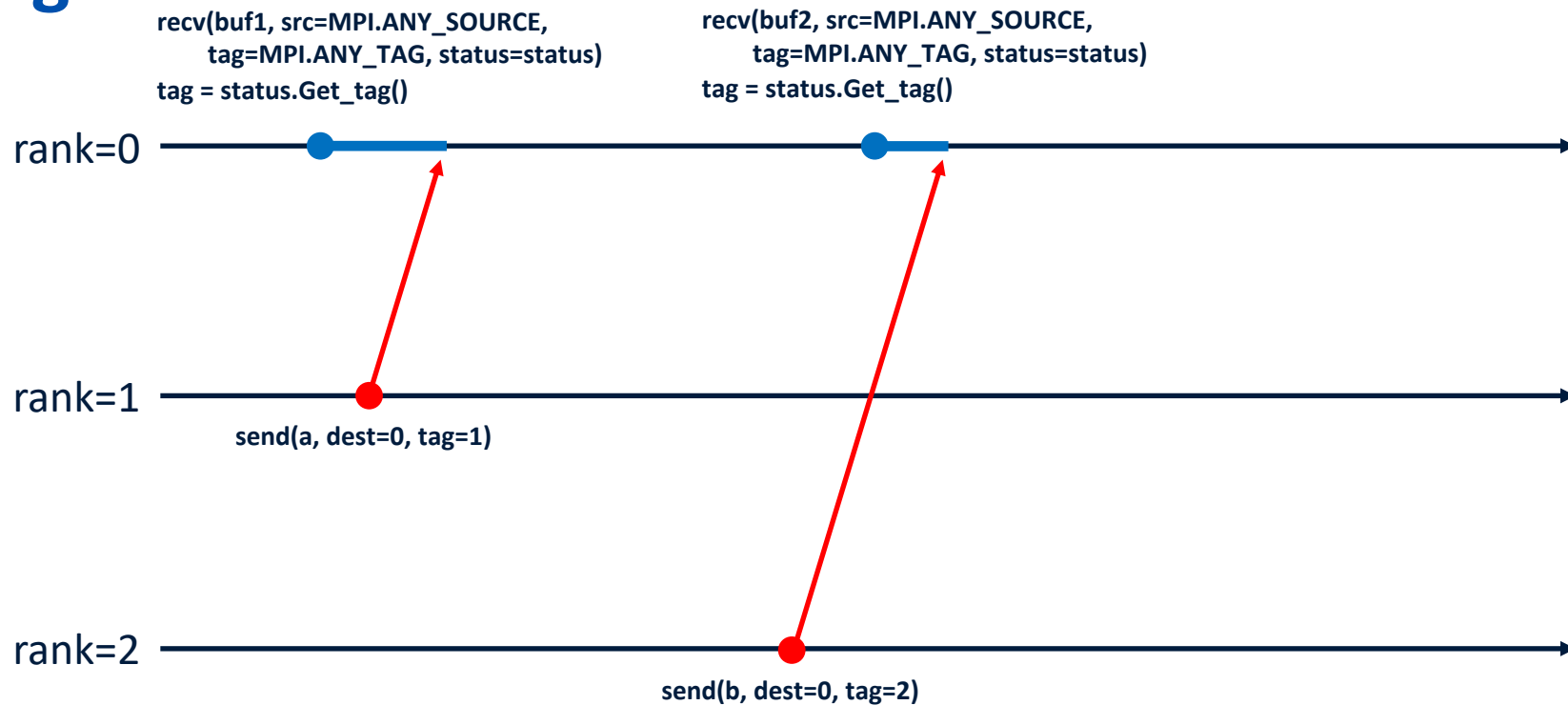


# Tags

Message buffering!



# Tags





# 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.