Lecture 04

Parallel universes

High Performance Computing for Data Science - SISSA, 2023-2024

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Outline

1. Parallel computing paradigms
    - Multithreading
    - Multiprocessing
    - MPI
2. GPU computing
3. Using HPC resources

Part of these notes is re-adapted from this lecture and this lecture (license) and this lecture (license).

Parallel computing paradigms

Introduction

Do you realize that you need more computational power than a single processor can provide? What steps should you take?

1. Profile your application to pinpoint the actual performance bottlenecks.
2. Is it possible to optimize these slow areas? Could you integrate an existing library to help?
3. Are there straightforward optimizations that could be implemented with minimal effort?
4. Consider using tools like Numba or Cython to speed up critical functions.
5. Explore options for parallelizing your code.

In scientific computing, there is often a need to parallelize code, either because running computations on a single core takes too long or because certain hardware (like supercomputers) requires code to be parallelized to operate.

Parallel computing paradigms (1/3)

Over the past ten years, the enhancement in CPU performance has largely been achieved through the addition of more cores, rather than through improvements in single-core performance. This trend emphasizes the importance of parallel processing, which leverages multiple CPU cores simultaneously, either through multithreading or multiprocessing.

Parallel computing is typically categorized into three main models:

1. **"Embarrassingly" parallel**: In this model, there is no need for synchronization or communication between instances. Multiple instances of the code can be run separately and their results combined later.

Parallel computing paradigms (2/3)

2. **Shared memory parallelism (multithreading)**:

- Threads perform separate tasks but communicate through shared memory and shared variables.
- Due to the Global Interpreter Lock (GIL) in Python, multiple threads within the same Python program cannot execute simultaneously, limiting the effectiveness of multithreading to I/O-bound tasks.
- External libraries written in languages like C, which are called from Python, can still effectively use multithreading.

Parallel computing paradigms (3/3)

3. **Distributed memory parallelism (multiprocessing)**:

- Each process manages its own memory segment and communicates with other processes as necessary through message passing.
- A single process can contain one or more threads.
- Processes can operate on different CPU cores or even on different computers.
- The creation and destruction of processes are more resource-intensive than thread management.
- Multiprocessing is particularly effective for CPU-bound tasks, which are computationally intensive.

Multithreading

Multithreading and the GIL

Python's design includes a mechanism known as the Global Interpreter Lock (GIL), which allows only one thread to execute Python bytecode at a time within a process. This design choice means that some common multithreading approaches effective in languages like C, C++, or Fortran may not be effective in Python. However, there are still advantages to Python's approach to parallelism:

- **External libraries**: Libraries such as NumPy, SciPy, and Pandas, which are written in C or other languages, can release the GIL and operate in a multi-threaded manner.
- **I/O operations**: Most input/output operations release the GIL, which is beneficial since I/O operations are generally slow. The Python threading library can be utilized to multithread these I/O operations effectively.
- **Circumventing the GIL**: Python libraries like `multiprocessing` and `mpi4py` facilitate running multiple Python processes, thereby circumventing the GIL and allowing parallel processing without the single-thread limitation.

Multithreading example (1/2)

Consider the following Python code, which performs a symmetrical matrix inversion on a large matrix using NumPy and measures the time taken for the operation:

```
import numpy as np
import time

# Generate a random 4000x4000 matrix and make it symmetrical.
A = np.random.random((4000, 4000))
A = A @ A.T

start_time = time.time()
np.linalg.inv(A)
end_time = time.time()

print("Time spent for inverting A is", round(end_time - start_time, 2), 's')
```

Multithreading example (2/2)

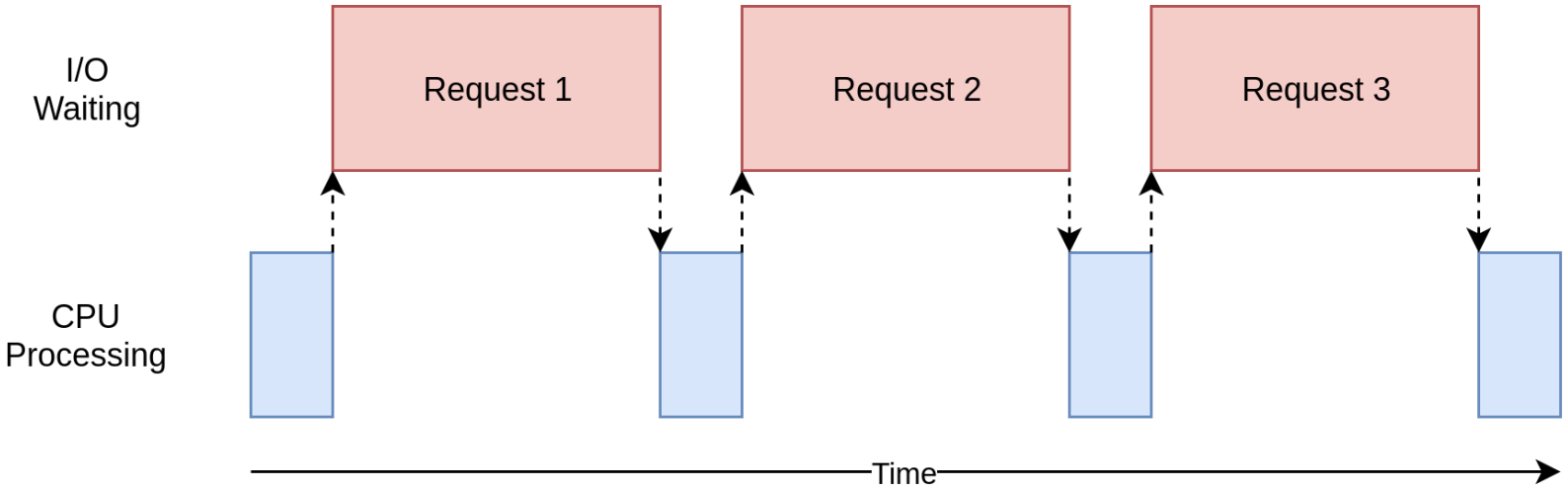
When this code is executed in a Jupyter notebook or a Python script, it will automatically utilize multithreading through OpenMP due to NumPy's configuration. This multithreading capability allows the matrix inversion to be completed more quickly by leveraging multiple CPU cores.

To run NumPy operations on a single thread, which typically leads to a longer runtime, you can set an environment variable to limit the number of threads used. The specific environment variable depends on NumPy's compilation settings on your system:

- For OpenMP implementations, use: `export OMP_NUM_THREADS=1`
- For Intel Math Kernel Library (MKL) implementations, use: `export MKL_NUM_THREADS=1`

Setting these variables forces NumPy to perform operations using only one thread, which can be useful for debugging or for comparing performance differences between single-threaded and multi-threaded operations.

Multithreaded I/O (1/2)



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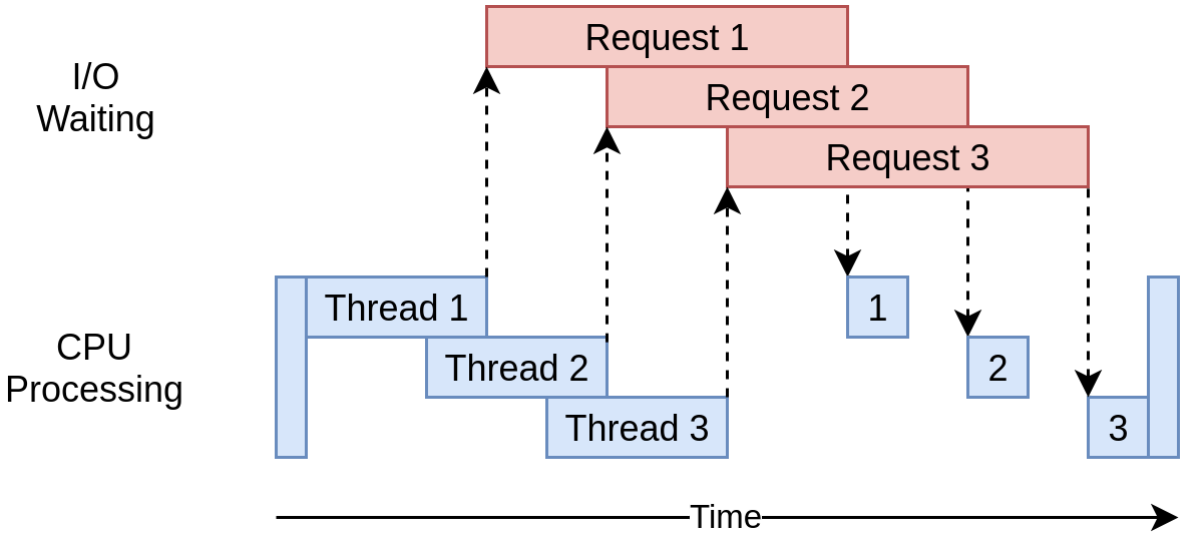
The `threading` library provides an API for creating and working with threads. The simplest approach to create and manage threads is to use the `ThreadPoolExecutor` class.

Multithreaded I/O (2/2)

```
import concurrent.futures

def download_all_sites(sites):
    with concurrent.futures.ThreadPoolExecutor(max_workers=4) as executor:
        executor.map(my_download_function, sites)
```



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Multiprocessing

Multiprocessing

The `multiprocessing` module in Python provides a means to create processes using an API similar to that of the `threading` module. By using subprocesses instead of threads, this module effectively circumvents the Global Interpreter Lock (GIL), as each subprocess runs as an independent Python process.

Multiprocessing example: using `Pool` objects (1/2)

One common approach to employing `multiprocessing` is through `Pool` objects, which can parallelize the execution of a function across multiple input values using the `Pool.map()` function, much like the threading approach.

```
import multiprocessing as mp

def square(x):
    return x * x

if __name__ == '__main__':
    nprocs = mp.cpu_count()  # Number of CPU cores.
    print(f"Number of CPU cores: {nprocs}")

    # Using a context manager to manage Pool resources.
    with mp.Pool(processes=nprocs) as pool:
        result = pool.map(square, range(20))
    print(result)
```

Multiprocessing example: using `Pool` objects (2/2)

This script calculates the square of numbers from 0 to 19 in parallel.

For functions that require multiple arguments, `Pool.starmap()` can be used.

```
import multiprocessing as mp

def power_n(x, n):
    return x ** n

if __name__ == '__main__':
    nprocs = mp.cpu_count()  # Number of CPU cores.
    print(f"Number of CPU cores: {nprocs}")

    with mp.Pool(processes=nprocs) as pool:
        result = pool.starmap(power_n, [(x, 2) for x in range(20)])
    print(result)
```

This example computes the power of numbers from 0 to 19 raised to the second power, demonstrating `Pool.starmap()`.

Interactive environments and limitations

In interactive environments like Jupyter, the `multiprocessing.Pool` might not function as expected because the `__main__` module needs to be importable by child processes. A fork of `multiprocessing`, called `multiprocess`, is recommended for use in such environments. All we have to do is install it by pip install `multiprocess` and change the import statement: `from multiprocess import Pool`.

The `multiprocessing` module also includes other functionalities like `Process` and `Queue`, which offer more control over individual processes.

MPI

Introduction to MPI

The Message Passing Interface (MPI) is a standardized and portable API used for communication among separate processes in a parallel computing environment. MPI offers exceptional portability and scalability, allowing the same code to run efficiently on both modest hardware and the most advanced supercomputers available.

Official MPI specifications provide C and Fortran interfaces, enhancing its adoption across various systems. For Python programmers, the unofficial `mpi4py` offers a convenient way to access MPI features.

Key features of MPI

MPI is known for its extensive functionality, with over 300 procedures, although a typical application might only use a few. Here's a look at some of the core features MPI supports:

- **Process communication**: MPI excels in sending and receiving messages, whether between two or multiple processes.
- **Synchronization**: It provides mechanisms to synchronize operations across different processes.
- **Communicator management**: Communicators in MPI are critical as they define a group of processes that will communicate with each other.
- **Advanced features**: MPI also supports advanced operations like creating custom data types, one-sided communications, and parallel I/O.

MPI execution model (1/2)

How MPI works

An MPI program launches as multiple independent, identical processes, potentially spread across different CPUs or even different machines. These processes are interconnected, usually requiring a high-bandwidth, low-latency network to function optimally.

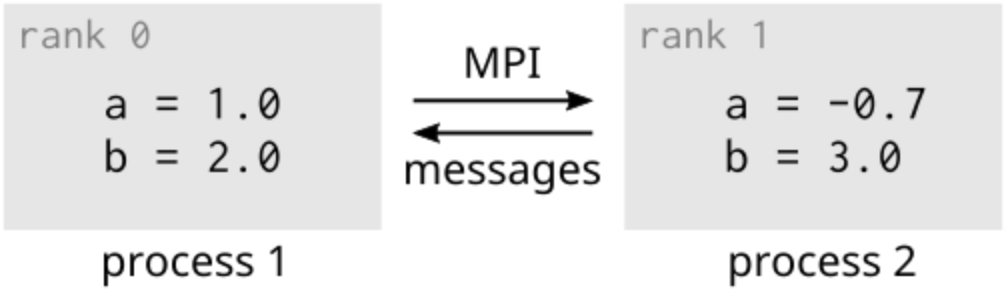
MPI rank and communicators

Each process in an MPI program is assigned a unique identifier known as a *rank*. Ranks enable differentiation of tasks among processes:

```
if rank == 0:
    # Task for rank 0.
elif rank == 1:
    # Task for rank 1.
else:
    # Tasks for all other ranks.
```

Data model

Since all MPI processes are completely independent, this means also a complete separation of data. Each process has its own separate memory space, i.e. all variables and data structures are local to the process. To exchange information, processes need to explicitly send and receive messages.



MPI execution model (2/2)

A *communicator* in MPI is a group of processes that can interact with each other. All MPI processes belong to a global communicator by default (`MPI_COMM_WORLD`), but custom communicators can also be defined.

For anyone beginning with MPI, understanding how to query the number of processes and their ranks is essential. These are typically done using `Get_size()` and `Get_rank()` methods of a communicator:

```
# hello.py
from mpi4py import MPI

comm = MPI.COMM_WORLD  # Global communicator
size = comm.Get_size()  # Number of processes
rank = comm.Get_rank()  # Unique identifier for this process

print(f"I am rank {rank} in a group of {size} processes.")
```

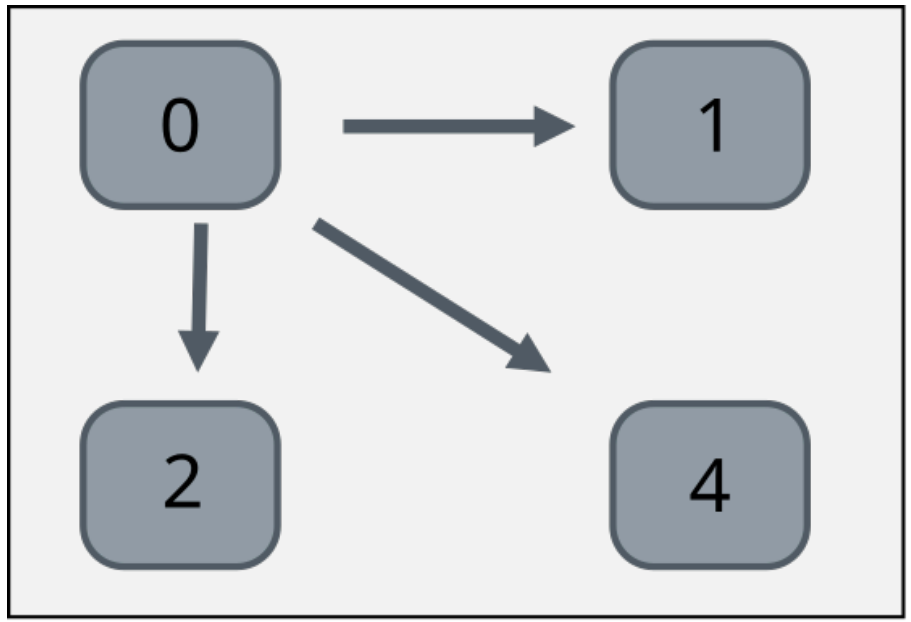
Running an MPI program

An MPI program is initiated using a launcher like `mpirun` or `mpiexec`, specifying the number of processes:

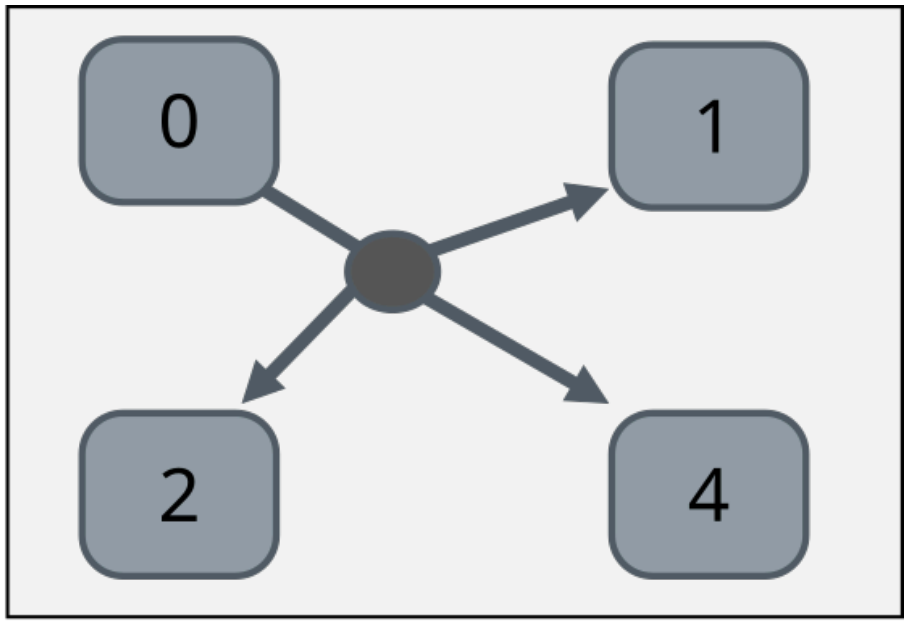
```
mpirun -np 4 python3 hello.py

I am rank 2 in group of 4 processes.
I am rank 0 in group of 4 processes.
I am rank 3 in group of 4 processes.
I am rank 1 in group of 4 processes.
```

MPI communication

MPI processes are independent, requiring explicit messaging for coordination. This communication falls into two categories: point-to-point and collective. While collective communication involves multiple processes simultaneously and will be covered later, our focus here is on point-to-point communication between two processes.



Point-to-point



Collective

Point-to-point communication

Point-to-point communication involves one process sending a message to another process, which receives it. The crucial aspect is that every send operation must have a corresponding receive operation, and these must match not only in timing but also in specifying the correct source and destination ranks.

Example: sending and receiving a dictionary

```
from mpi4py import MPI

comm = MPI.COMM_WORLD
rank = comm.Get_rank()

if rank == 0:
    data = {'a': 7, 'b': 3.14}
    comm.send(data, dest=1, tag=0)
elif rank == 1:
    data = comm.recv(source=0, tag=0)
```

Mechanics of sending and receiving

In MPI with Python, you can use `send()` and `recv()` methods from a communicator to exchange Python objects that are serializable via pickle. This includes most Python standard and derived objects.

- `send(data, dest, tag)`: Sends `data` to the process with rank `dest` with a given `tag`.
- `recv(source, tag)`: Receives data with tag `tag` from the process with rank `source`. The data is returned as the function's result.

These operations are **blocking**; they do not complete until it's safe to use the involved memory, necessitating successful coordination with the matching operation in the other process. Mismanagement can lead to deadlocks, where processes wait indefinitely for each other to send or receive data.

Communication patterns

Pairwise exchange

Pipe, a ring of processes exchanging data

Fast communication of large arrays

While MPI for Python allows for the sending and receiving of general Python objects, this flexibility can lead to performance issues due to the need to serialize and deserialize (pickle and unpickle) objects. For more efficient communication, especially of large data sets like NumPy arrays, MPI for Python provides specialized routines.

Efficient NumPy array communication

The efficient communication of large arrays, such as NumPy arrays, utilizes routines in MPI for Python designed specifically for contiguous memory buffers, which avoid the overhead of serialization.

Sending and receiving arrays

Using the upper case `Send()` and `Recv()` methods allows for direct memory copying, which is significantly faster for large data transfers. This works for *buffer*-like data, like strings and NumPy arrays.

Example of sending a NumPy array:

```
from mpi4py import MPI
import numpy

comm = MPI.COMM_WORLD
rank = comm.Get_rank()

data = numpy.empty(100, dtype=float)
if rank == 0:
    data[:] = numpy.arange(100, dtype=float)
    comm.Send(data, dest=1)
elif rank == 1:
    comm.Recv(data, source=0)
```

Combined Send and Receive

MPI also supports combined send and receive operations, which can reduce the risk of deadlocks:

```
from mpi4py import MPI
import numpy

comm = MPI.COMM_WORLD
rank = comm.Get_rank()

data = numpy.arange(10, dtype=float) * (rank + 1)
buffer = numpy.empty(10, float)

if rank == 0:
    tgt, src = 1, 1
elif rank == 1:
    tgt, src = 0, 0

comm.Sendrecv(data, dest=tgt, recvbuf=buffer, source=src)
```

Manual buffer definition

```
from mpi4py import MPI
import numpy

comm = MPI.COMM_WORLD
rank = comm.Get_rank()

data = numpy.empty(100, dtype=float)
if rank == 0:
    data[:] = numpy.arange(100, dtype=float)
    comm.Send([data, 100, MPI.DOUBLE], dest=1)
elif rank == 1:
    comm.Recv([data, 100, MPI.DOUBLE], source=0)
```

This approach allows for communication of any type of contiguous data array using MPI's capabilities for high-performance data transfers.

Non-blocking communication

MPI offers non-blocking communication routines that allow communication to occur in the background while the main program continues its execution. This approach can lead to more efficient code by overlapping computation with communication and reducing potential deadlocks.

Key concepts

- **Non-blocking methods**: Functions like `isend`, `irecv`, `Isend`, etc., start communication but return immediately, letting the program continue while the operation completes in the background.
- **Request objects**: Non-blocking calls return a `Request` object, which is used to manage and check the status of the ongoing communication.

Managing non-blocking communications (1/2)

Finalizing communications

Non-blocking communications must be finalized using one of the following methods:

- `wait()`: A blocking call that waits for the specific communication to complete.
- `test()`: A non-blocking call that checks if the communication has finished and returns a boolean value.

Managing non-blocking communications (2/2)

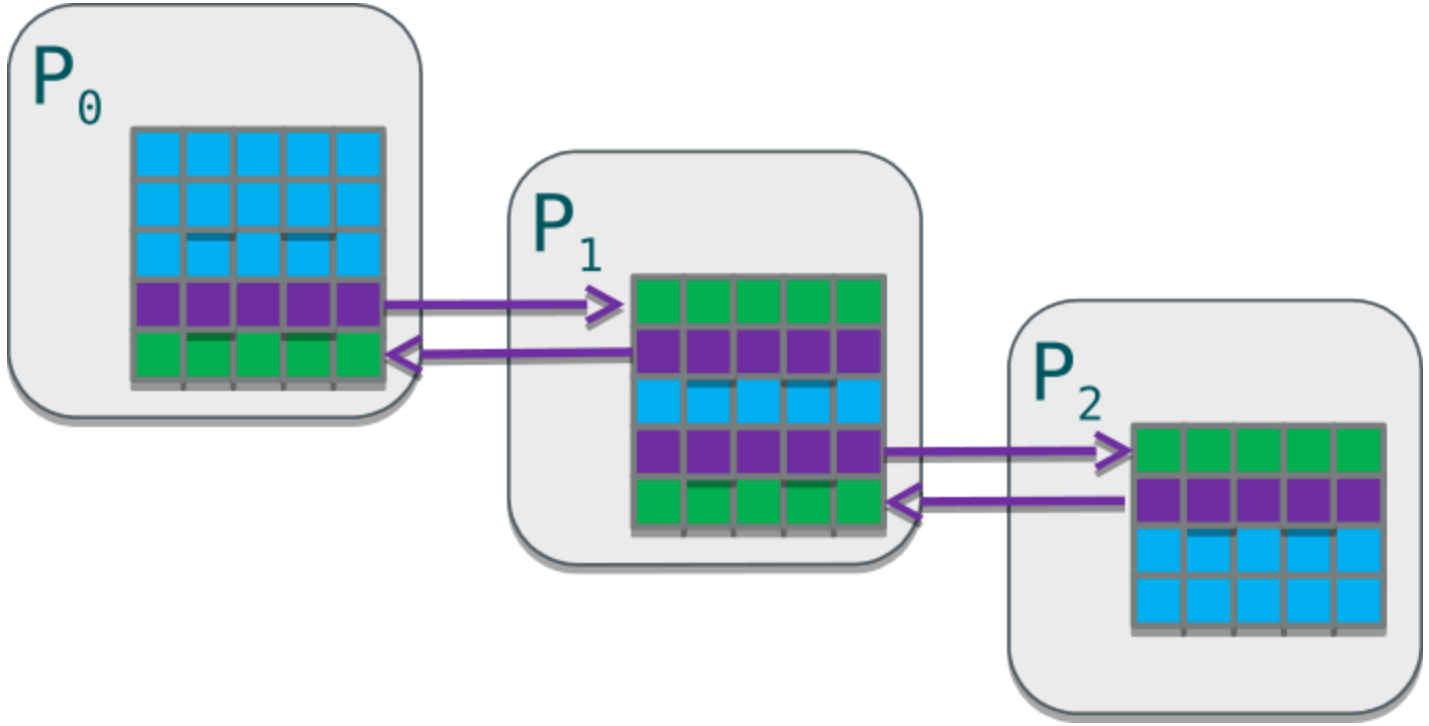
```
from mpi4py import MPI
import numpy

comm = MPI.COMM_WORLD
rank = comm.Get_rank()
size = comm.Get_size()

if rank == 0:
    data = numpy.arange(size, dtype=float) * (rank + 1)
    req = comm.Isend(data, dest=1, tag=0)
    # Other computations can be done here.
    req.wait()  # Wait for the send to complete.

elif rank == 1:
    data = numpy.empty(size, dtype=float)
    req = comm.Irecv(data, source=0, tag=0)
    # Other computations can be done here.
    req.wait()  # Wait for the receive to complete.
```

Handling multiple non-blocking operations

```
from mpi4py import MPI
import numpy

comm = MPI.COMM_WORLD
rank = comm.Get_rank()
size = comm.Get_size()

data = numpy.arange(10, dtype=float) * (rank + 1)
buffer = numpy.zeros(10, dtype=float)

tgt = rank + 1 if rank < size - 1 else MPI.PROC_NULL
src = rank - 1 if rank > 0 else MPI.PROC_NULL

req = [comm.Isend(data, dest=tgt), comm.Irecv(buffer, source=src)]

MPI.Request.waitall(req)  # Wait for all requests to complete.
```

Overlapping computation and communication

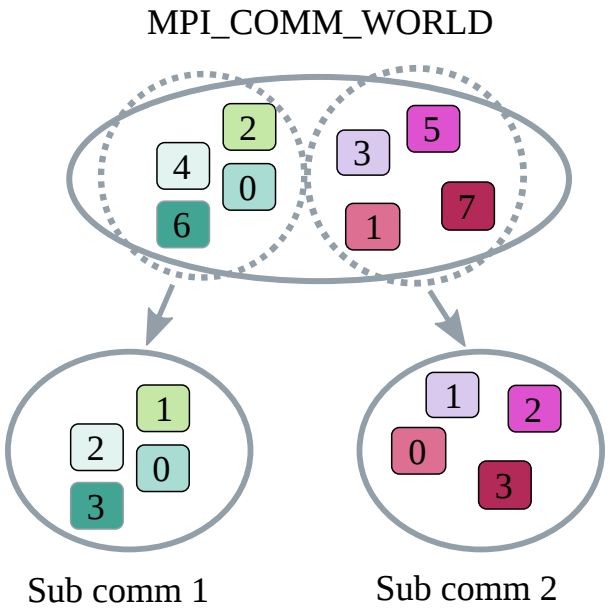
Non-blocking communication can be effectively utilized to overlap data transfer with computation, enhancing the efficiency of parallel programs.



Communicators in MPI

In MPI, a *communicator* is a fundamental object that groups processes for communication. It specifies the context in which MPI routines execute, allowing coordinated communication among sets of processes.

Each MPI process is part of a communicator and has a unique identifier (rank) within that communicator. Communicators dictate the scope and grouping of processes for communication tasks.



User-defined communicators

While all processes initially belong to the default global communicator `MPI.COMM_WORLD`, MPI also allows the creation of custom communicators to better control communication flows and groupings.

Creating custom communicators

A common use case for creating a custom communicator is to divide a large set of processes into smaller, more manageable groups based on certain criteria.

Example: splitting communicators

```
from mpi4py import MPI

comm = MPI.COMM_WORLD
rank = comm.Get_rank()

# Split processes by color grouping based on rank.
color = rank % 4
local_comm = comm.Split(color)
local_rank = local_comm.Get_rank()

print(f"Global rank: {rank} Local rank: {local_rank}")
```

In this example, processes are divided into four groups (colors 0-3). Each group forms a new communicator, and within each, the processes are reassigned ranks starting from zero.

Advantages of user-defined communicators

- **Isolation**: Custom communicators can isolate communication within specific groups of processes, improving efficiency and reducing interference.
- **Flexibility**: They allow more flexible management of processes based on the application's needs, such as dividing tasks that require different communication patterns.

Collective communication: one to many

Collective communication in MPI facilitates data transfers among all processes within a communicator, streamlining data movement, collective computations, and synchronization. This type of communication requires involvement from all processes in the communicator, ensuring that data is uniformly sent or received.

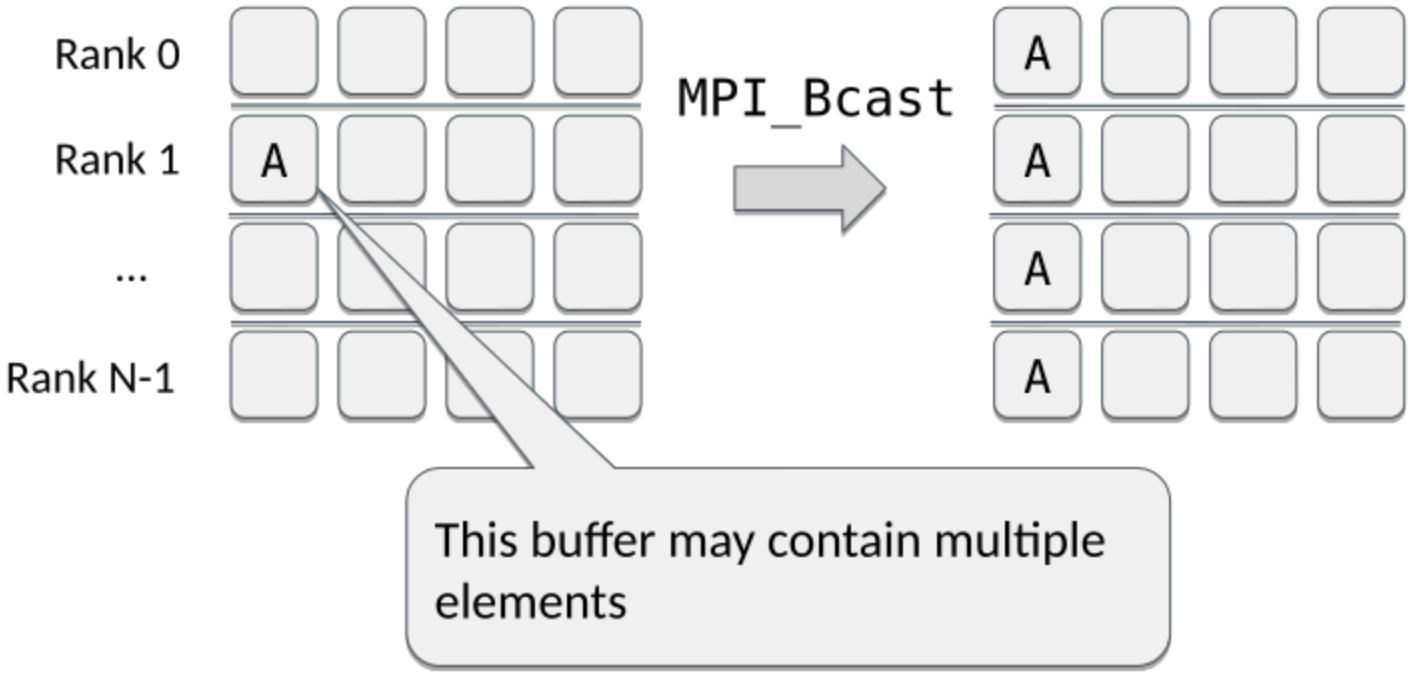
Benefits

- **Efficiency**: Collective communication is generally more efficient than equivalent point-to-point operations.
- **Simplicity**: It simplifies code, making it easier to maintain and understand.

Communication Patterns

Broadcast

The `Broadcast` or `Bcast` operation shares data from one process (the root) to all other processes in the communicator.

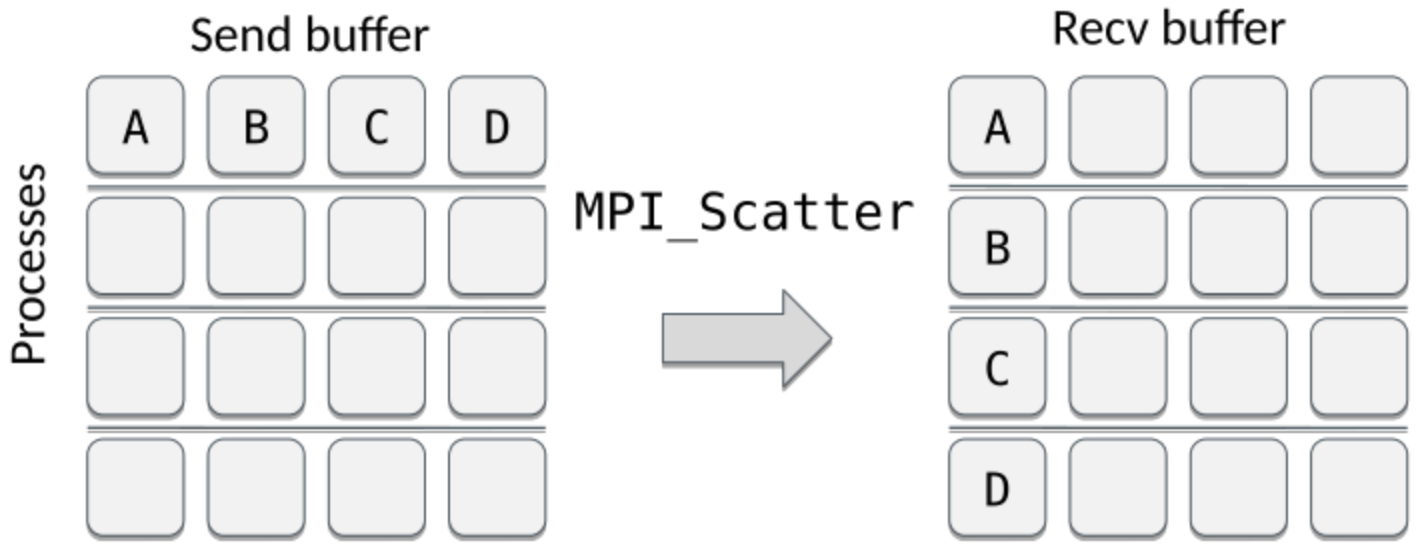


Example: broadcasting data

```
from mpi4py import MPI
import numpy

comm = MPI.COMM_WORLD
rank = comm.Get_rank()

if rank == 0:
    py_data = {'key1': 0.0, 'key2': 11}  # Python dictionary.
    data = numpy.arange(8) / 10.0        # NumPy array.
else:
    py_data = None
    data = numpy.zeros(8)

# Broadcast Python dictionary.
new_data = comm.bcast(py_data, root=0)
# Broadcast NumPy array.
comm.Bcast(data, root=0)
```

Scatter

The `Scatter` operation divides data from one process and distributes it among all processes in the communicator.



Example: scattering data

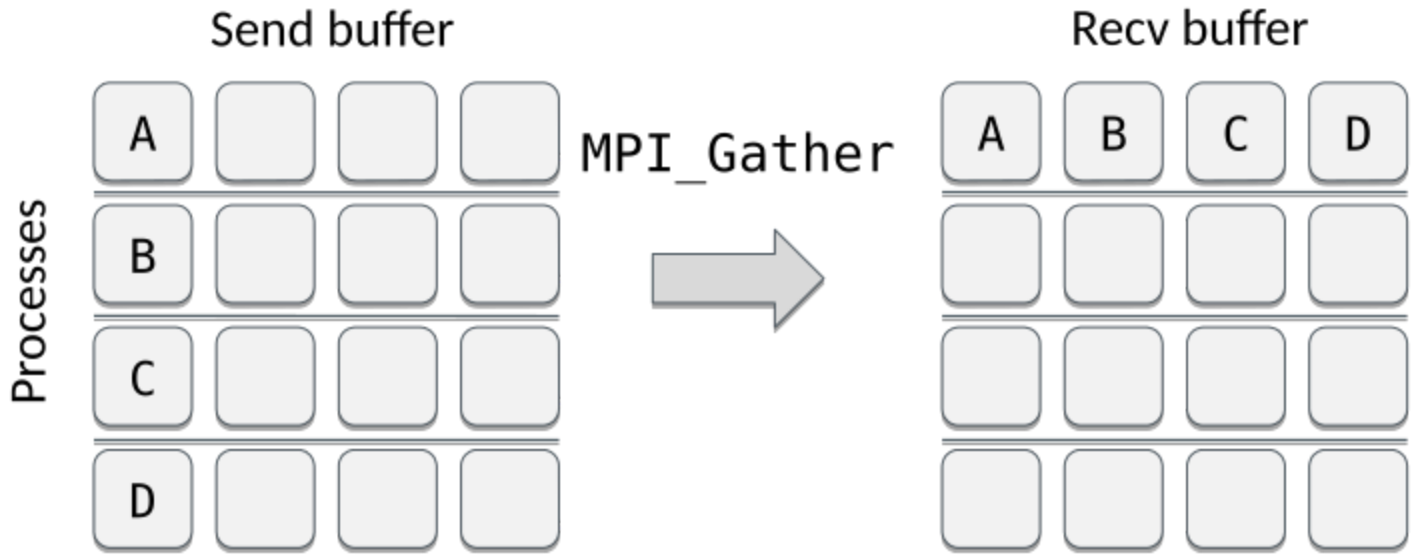
```
from mpi4py import MPI
import numpy

comm = MPI.COMM_WORLD
rank = comm.Get_rank()
size = comm.Get_size()

if rank == 0:
    py_data = list(range(size))  # List of integers.
    data = numpy.arange(size**2, dtype=float)  # NumPy array.
else:
    py_data = None
    data = None

# Scatter list of integers.
new_data = comm.scatter(py_data, root=0)
# Prepare a buffer for scattering NumPy array.
buffer = numpy.empty(size, dtype=float)
# Scatter NumPy array.
comm.Scatter(data, buffer, root=0)
```

Collective communication: many to one

Collective communication routines in MPI not only facilitate data distribution but also collection from multiple processes to a single one. This discussion covers two primary MPI operations that enable such data collection: `Gather` and `Reduce`.

Gather operation

The `Gather` operation collects data from all processes in the communicator and delivers it to a single designated process (root).

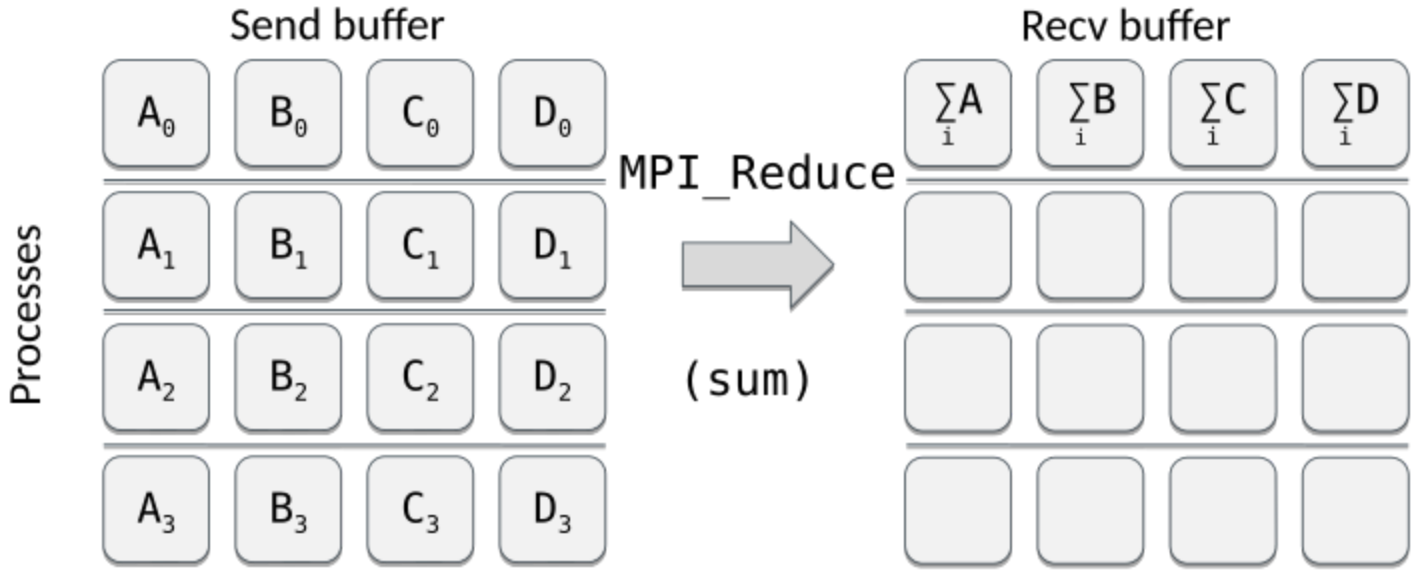


Example: gathering data

```
from mpi4py import MPI
import numpy

comm = MPI.COMM_WORLD
rank = comm.Get_rank()
size = comm.Get_size()

# Each process generates data based on its rank.
data = numpy.arange(10, dtype=float) * (rank + 1)
# Buffer for gathering data at root.
buffer = numpy.zeros(size * 10, dtype=float)

# Gather single values from each process.
n = comm.gather(rank, root=0)
# Gather arrays from each process.
comm.Gather(data, buffer, root=0)
```

Reduce operation

The `Reduce` operation collects data from all processes, applies a specified operation (like sum, max, min), and stores the result in one process.



Example: reducing data

```
from mpi4py import MPI
import numpy

comm = MPI.COMM_WORLD
rank = comm.Get_rank()
size = comm.Get_size()

# Data array influenced by rank.
data = numpy.arange(10 * size, dtype=float) * (rank + 1)
# Buffer for reduced data at root.
buffer = numpy.zeros(size * 10, dtype=float)

# Sum all ranks.
n = comm.reduce(rank, op=MPI.SUM, root=0)
# Sum all data arrays.
comm.Reduce(data, buffer, op=MPI.SUM, root=0)
```

Variants and flexibility

MPI also offers variations like `Scatterv` and `Gatherv` for operations involving variable amounts of data per process, enhancing flexibility in data distribution and collection.

Collective communication: many to many

Collective communication in MPI not only involves one-to-one or many-to-one communications but also encompasses global interactions among all processes within a communicator. While these global communications are resource-intensive, they are crucial for certain parallel algorithms.

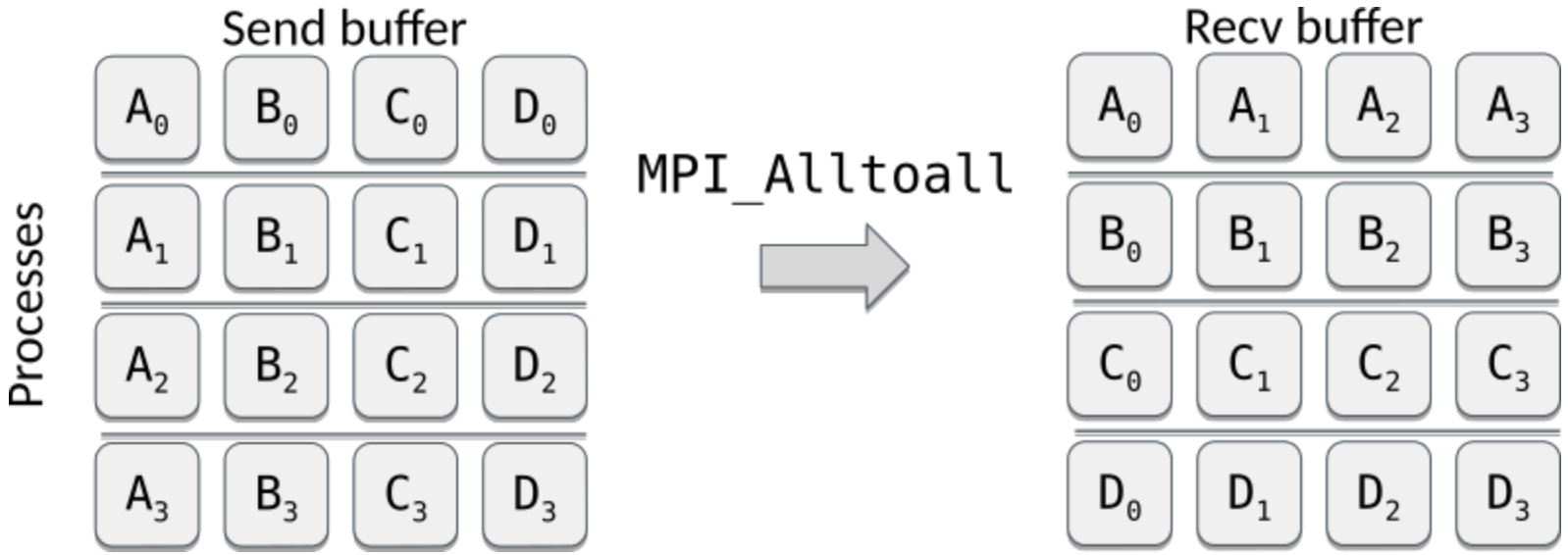
Key operations

Allreduce combines the functionalities of Reduce and Broadcast. It performs a reduction operation (like sum, max, etc.) on data from all processes and then distributes the result back to all processes.

```
from mpi4py import MPI
import numpy as numpy

comm = MPI.COMM_WORLD
rank = comm.Get_rank()
size = comm.Get_size()

# Data array influenced by rank.
data = numpy.arange(10 * size, dtype=float) * (rank + 1)
buffer = numpy.empty(size * 10, dtype=float)

# Allreduce operation.
result = comm.allreduce(rank, op=MPI.SUM)
comm.Allreduce(data, buffer, op=MPI.SUM)
```

Key operations

Alltoall allows each process to send and receive data to and from every other process, effectively performing a matrix transpose of the data.



Example: Alltoall Operation

```
from mpi4py import MPI
import numpy as numpy

comm = MPI.COMM_WORLD
rank = comm.Get_rank()
size = comm.Get_size()

# Prepare data.
py_data = list(range(size))
data = numpy.arange(size**2, dtype=float)

# Perform Alltoall.
new_data = comm.alltoall(py_data)

buffer = numpy.zeros_like(data)
comm.Alltoall(data, buffer)
```

Common mistakes in collective communication

1. **Incorrect conditional call**: Collective operations should not be called conditionally within a subset of processes.

   ```
   if rank == 0:
       comm.bcast(...)
   ```

   This is incorrect because all processes must participate in the collective operation.

2. **Assuming synchronization**: Collective operations do not guarantee that all processes exit the call simultaneously. They only ensure that it is safe to proceed with the data.

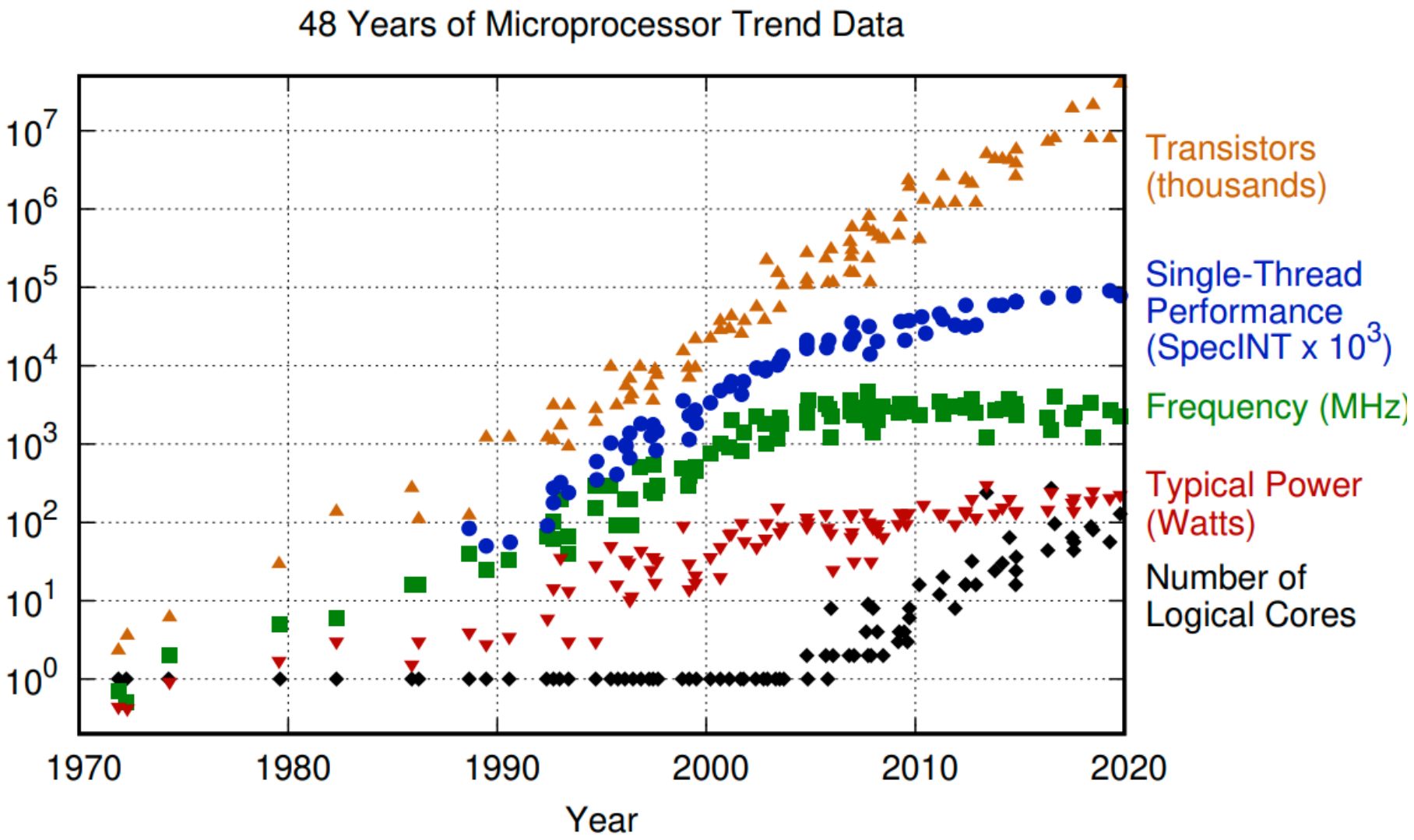
3. **Buffer mismanagement**: Using the same buffer for both input and output can lead to unexpected results.

   ```
   comm.Scatter(a, a, MPI.SUM)
   ```

   Use separate buffers for input and output to avoid overwriting data prematurely.

GPU computing

Moore's law and the shift to multicore processing



Original data up to the year 2010 collected and plotted by M. Horowitz, F. Labonte, O. Shacham, K. Olukotun, L. Hammond, and C. Batten
New plot and data collected for 2010-2019 by K. Rupp

Moore's law and the shift to multicore processing

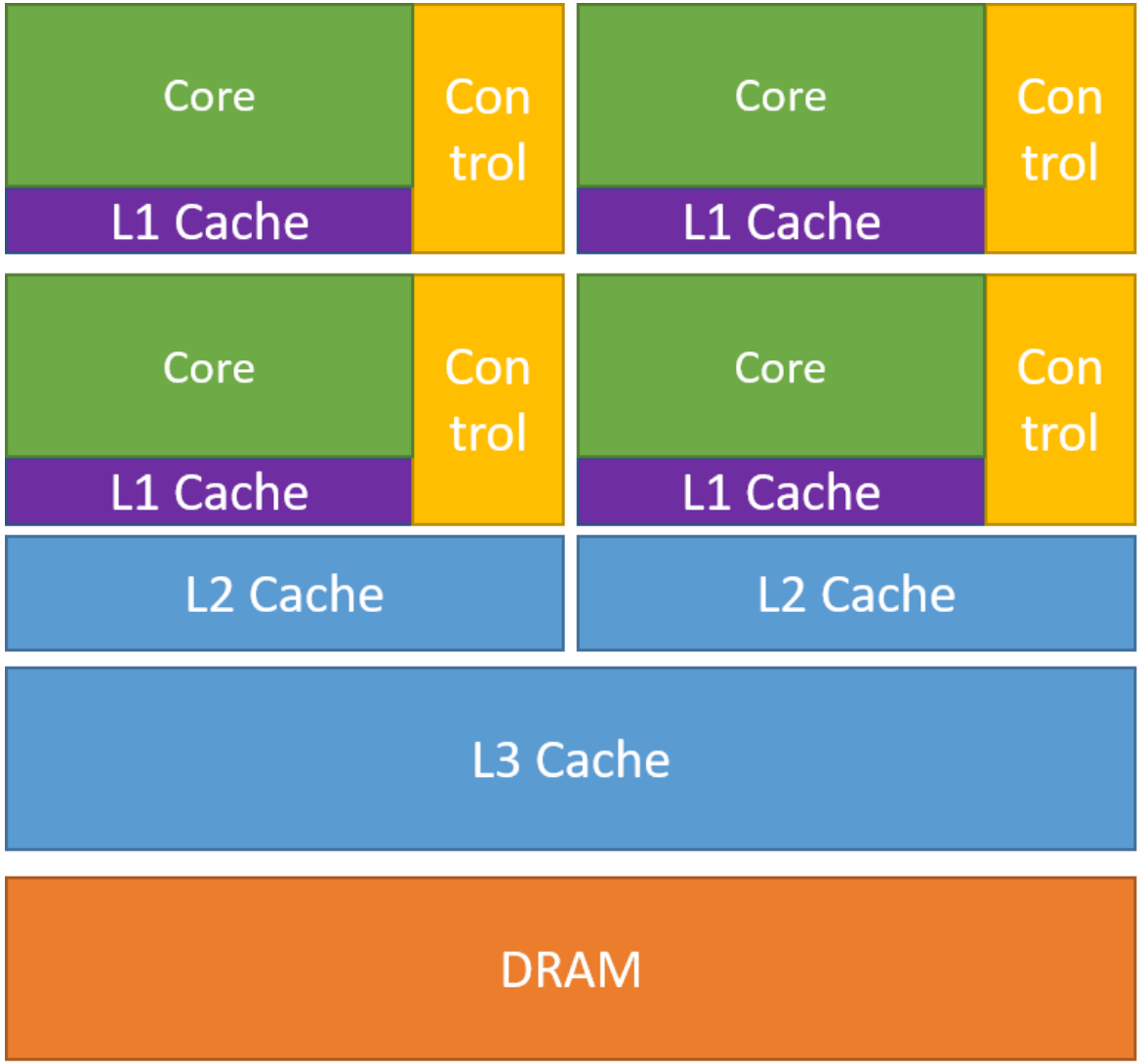
Moore's law suggests that the number of transistors on a chip doubles approximately every two years. However, due to power consumption limits, the increase in core frequency has stagnated, pushing the shift towards multicore processors around the mid-2000s to maintain performance growth.

Why use GPUs?

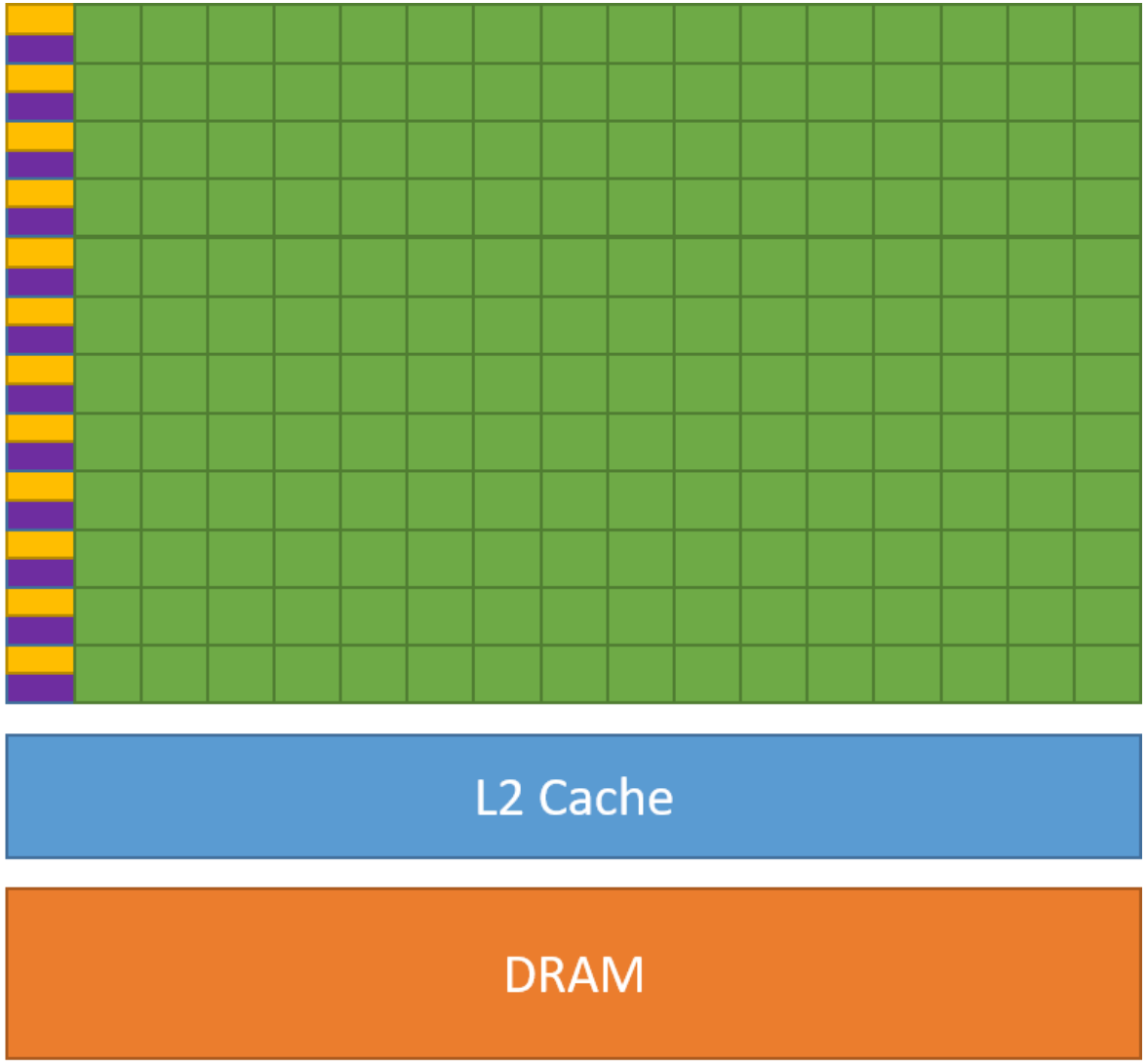
GPUs, initially designed for rendering graphics, have evolved into powerful accelerators for general computational tasks. They offer significantly higher instruction throughput and memory bandwidth within a similar price and power envelope compared to CPUs.

This section explores why and how to utilize GPUs for computing, focusing on their architecture, programming models, and appropriate use cases.

Differences between CPUs and GPUs (1/2)



CPU



GPU

Differences between CPUs and GPUs (2/2)

CPU	GPU
General purpose	Highly specialized for parallelism
Good for serial processing	Good for parallel processing
Excellent for task parallelism	Excellent for data parallelism

- GPUs manage many threads in parallel.
- The CPU controls workflow and data transfers.
- Efficient GPU use requires problem decomposition into concurrently runnable parts.

Performance strategies

Historically, performance gains in computer architecture have come from either boosting single-processor speeds or, more recently, increasing the number of physical cores.

GPU architecture and programming model

Understanding GPU architecture and its programming model is essential for leveraging its capabilities effectively:

GPU terminology

- **Host**: CPU
- **Device**: GPU
- **Kernels**: Functions executed on the GPU, launched by the host.

GPU structure (1/3)

1. Streaming Multiprocessors (SMs)

A GPU consists of several SMs, each being a core computational unit capable of executing multiple concurrent threads. The number of SMs can vary depending on the GPU model and architecture (for example, NVIDIA's different architectures like Volta, Turing, Ampere). Each SM includes:

- **Core processors**: For actual data processing.
- **Special functional units**: Like tensor cores for deep learning and ray tracing cores for graphics.
- **Local memory**: Registers and shared memory accessible by all threads within the SM.
- **Control units**: For managing thread execution.

GPU structure (2/3)

2. Blocks (or Thread Blocks)

Each block, or thread block, is a group of threads that execute together on a single SM. Blocks are a key component of GPU programming models like CUDA and OpenCL. Here's why they are organized into blocks:

- **Shared memory access**: Threads within the same block can share data through a shared memory, which is much faster than accessing global memory. This reduces memory latency and increases throughput.
- **Synchronization**: Threads in the same block can synchronize their operations using barriers. This is useful for operations that depend on certain computations to be completed before proceeding.
- **Resource allocation**: Managing resources at the block level helps in balancing load across SMs and optimizes the usage of the GPU’s computational resources.

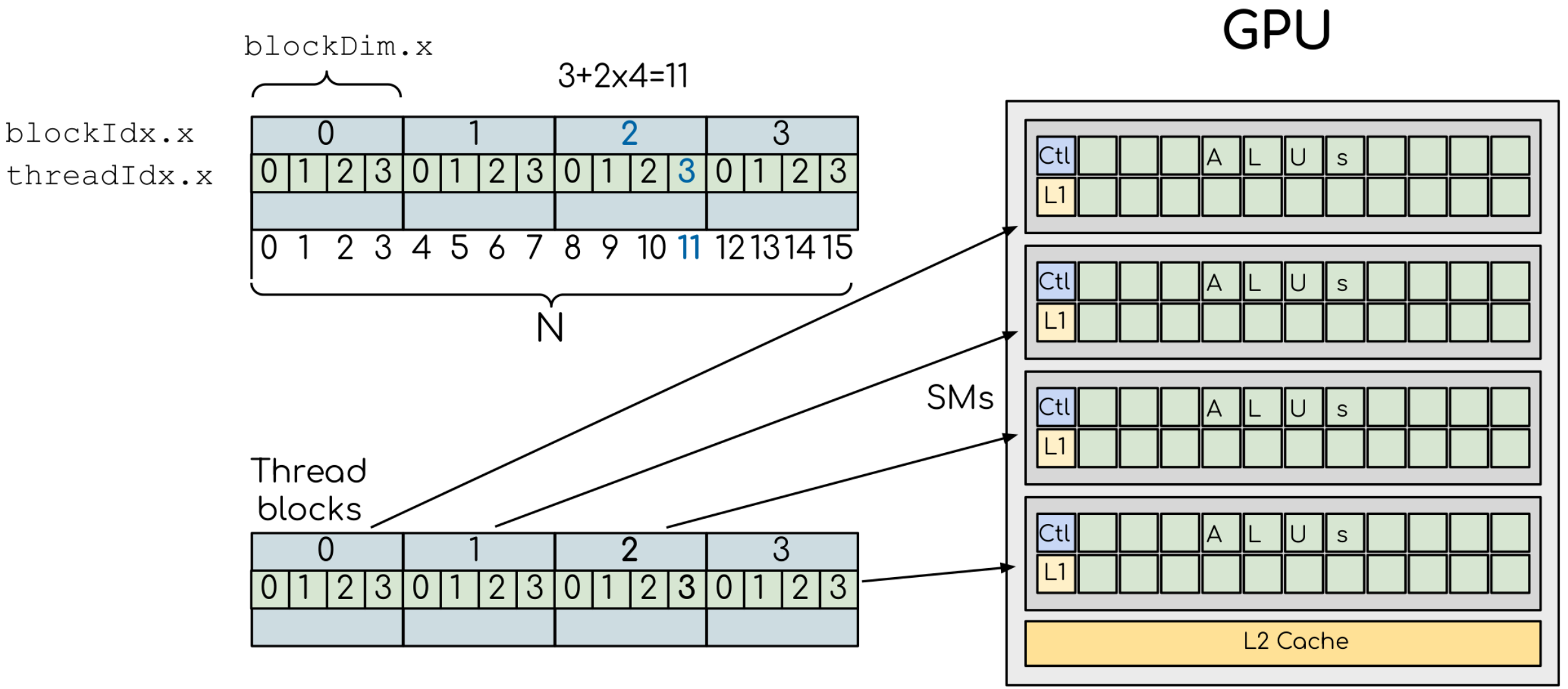
GPU structure (3/3)

3. Threads

Threads are the smallest execution units in a GPU. Each thread runs a small set of instructions on its own set of data. The massive number of threads a GPU can handle allows for detailed and complex computations to be broken down into simpler, parallel tasks. Threads in GPUs are:

- **Lightweight**: Designed to be extremely lightweight to allow thousands to run in parallel with minimal overhead.
- **Interchangeable**: Since each thread performs the same operation on different data, they can be scheduled and executed in any order relative to other threads, making GPU scheduling very flexible.

Thread hierarchy



Example

The NVIDIA A100 is based on the Ampere architecture, providing enhancements over the Volta architecture used in the V100. Key specifications include:

- **Streaming Multiprocessors (SMs)**: The A100 features 108 SMs in its most typical data center configuration.
- **CUDA cores**: Each SM has 64 CUDA cores, totaling 6,912 CUDA cores.
- **Tensor Cores**: The A100 has more powerful Tensor Cores with new features and there are 4 Tensor Cores per SM, totaling 432 Tensor Cores.

Python on GPU

Significant advancements have been made in Python for GPU utilization, though it is still evolving.

For instance, CUDA is the programming model developed by NVIDIA for GPU programming.

Libraries

- **CuPy**: A NumPy/SciPy-compatible array library for GPU, easy to adopt for NumPy users.
- **cuDF**: Part of the RAPIDS suite, cuDF manipulates data frames on GPU with a pandas-like API.
- **PyCUDA**: Provides access to NVIDIA's CUDA programming API but requires knowledge of CUDA.
- **Numba**: Allows JIT compilation of Python code for execution on the GPU.

Numba for GPU programming

Numba is a just-in-time compiler for Python that allows using GPU directly by compiling Python code into kernels that can run on the GPU. This simplifies GPU programming by abstracting away many of the complexities.

Example: using Numba for vector addition

```
from numba import vectorize, cuda
import numpy as np

@vectorize(['float32(float32, float32)'], target='cuda')
def add_vectors(a, b):
    return a + b

# Create data.
a = np.array([1, 2, 3], dtype=np.float32)
b = np.array([4, 5, 6], dtype=np.float32)

# Compute result.
c = add_vectors(a, b)
```

Example: using Numba for matrix-matrix multiplication

```
import numpy as np
import numba

#@numba.guvectorize(['(float64[:,:], float64[:,:], float64[:,:])'], '(m,l),(l,n)->(m,n)', target='cuda')
@numba.guvectorize([numba.void(numba.float64[:,:], numba.float64[:,:], numba.float64[:,:])], '(m,l),(l,n)->(m,n)', target='cuda')
def matmul_numba_gpu(A, B, C):
    for i in range(A.shape[0]):
        for j in range(B.shape[1]):
            tmp = 0.0
            for k in range(B.shape[0]):
                tmp += A[i, k] * B[k, j]
            C[i,j] += tmp
```

- **Complexity and power**: `@vectorize` is simpler and designed for element-by-element operations. `@guvectorize` is more powerful and flexible, designed for operations that span multiple elements and possibly multiple dimensions.
- **Use cases**: Use `@vectorize` for simple, scalar output operations and `@guvectorize` for more complex array operations that might involve slicing, dicing, or reductions across dimensions.

Best practices for GPU computing

While GPUs are powerful, they require careful management of memory and computation strategies to be used effectively:

- **Memory transfers**: Data transfers between host and device should be minimized as they can become bottlenecks.
- **Execution strategy**: Kernels should be designed to maximize the occupancy of the GPU to improve performance.
- **Number of blocks per SM**: Typically, starting with 2 to 4 blocks per SM is a good baseline. Adjust based on your application's specific needs and profiling results.
- **Warp efficiency**: Since a warp consists of 32 threads, it is generally efficient to choose a block size (i.e. number of threads per block) that is a multiple of 32 to avoid partially filled warps, which can result in wasted GPU resources.

Using HPC resources

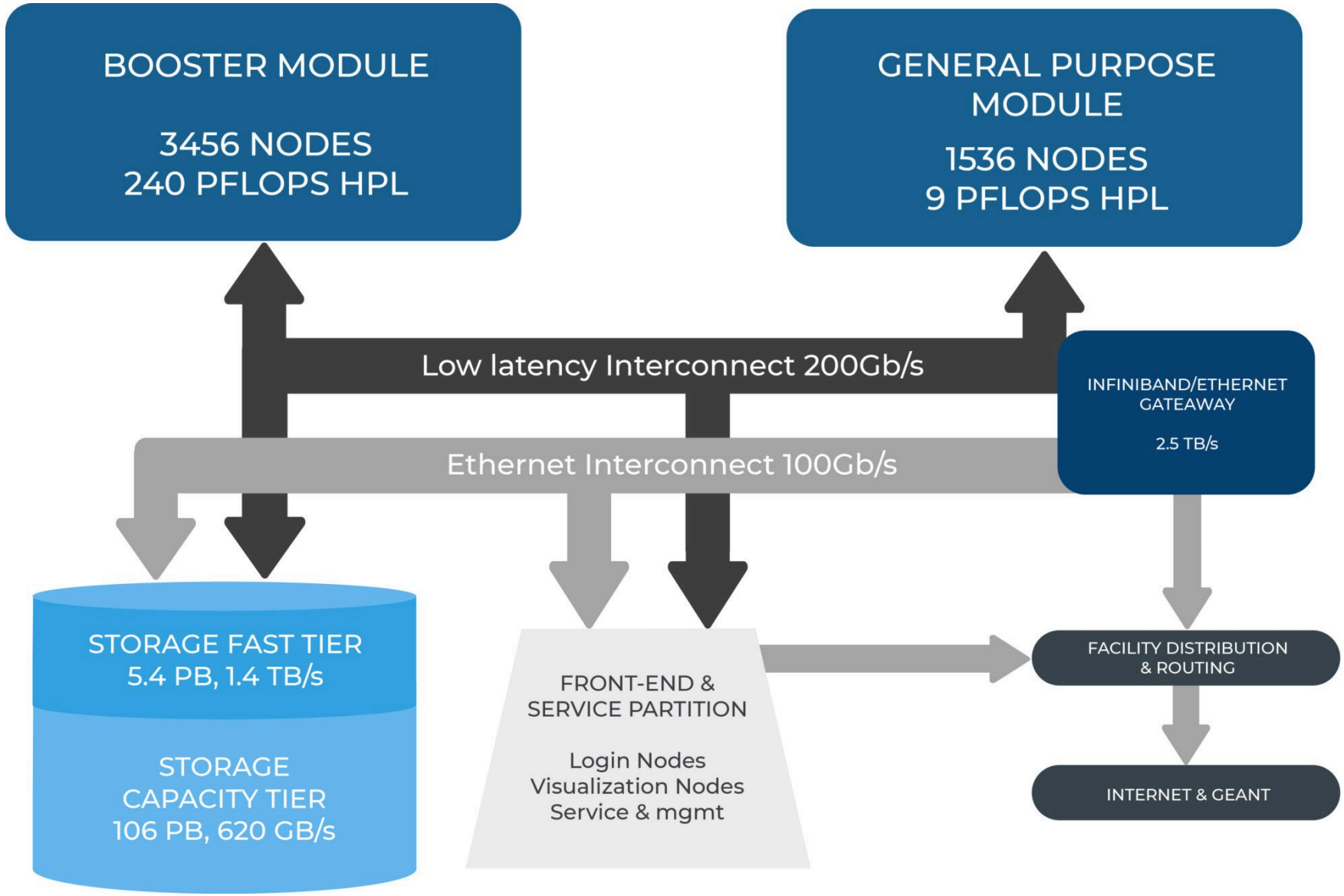
TOP10 System - November 2023

R_{max} and R_{peak} values are in PFlop/s. For more details about other fields, check the TOP500 description.

R_{peak} values are calculated using the advertised clock rate of the CPU. For the efficiency of the systems you should take into account the Turbo CPU clock rate where it applies.

Rank	System	Cores	Rmax (PFlop/s)	Rpeak (PFlop/s)	Power (kW)
1	**Frontier** - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE DOE/SC/Oak Ridge National Laboratory United States	8,699,904	1,194.00	1,679.82	22,703
2	**Aurora** - HPE Cray EX - Intel Exascale Compute Blade, Xeon CPU Max 9470 52C 2.4GHz, Intel Data Center GPU Max, Slingshot-11, Intel DOE/SC/Argonne National Laboratory United States	4,742,808	585.34	1,059.33	24,687
3	**Eagle** - Microsoft NDv5, Xeon Platinum 8480C 48C 2GHz, NVIDIA H100, NVIDIA Infiniband NDR, Microsoft Microsoft Azure United States	1,123,200	561.20	846.84	
...					
6	**Leonardo** - BullSequana XH2000, Xeon Platinum 8358 32C 2.6GHz, NVIDIA A100 SXM4 64 GB, Quad-rail NVIDIA HDR100 Infiniband, EVIDEN EuroHPC/CINECA Italy	1,824,768	238.70	304.47	7,404

Cineca Leonardo: system architecture



SLURM tutorial

SLURM (Simple Linux Utility for Resource Management) is a powerful cluster management and job scheduling system. In this tutorial, we will explore how to use SLURM for high performance computing, which is crucial for running computationally intensive tasks.

Basic SLURM commands

Here's a brief overview of basic SLURM commands you'll need:

- `sinfo`: View the status of nodes and partitions.
- `squeue`: Check the queue status and see all jobs currently scheduled on the cluster.
- `sbatch`: Submit a job script to the SLURM scheduler.
- `scancel`: Cancel a job.
- `srun`: Run a job interactively.

Writing a job script file

A job script tells SLURM what resources your job will need and the commands to execute the job. Below is an example script that requests GPU resources and runs a Python script using GPUs.

Here's a simple job script (`my_job.sh`) to run a Python script using SLURM:

```
#!/bin/bash
#SBATCH --job-name=gpu-test           # Job name.
#SBATCH --partition=gpu               # Partition (job queue).
#SBATCH --nodes=1                     # Number of nodes.
#SBATCH --ntasks-per-node=1           # Number of parallel tasks per node.
#SBATCH --mem=4G                      # Memory needed.
#SBATCH --time=00-00:15:00            # Time limit days-hrs:min:sec.
#SBATCH --output=gpu-test_%j.log      # Standard output and error log.

module load python/3.8                # Load Python module.
module load cuda/10.2                 # Load CUDA module, adjust as per your cluster setup.

python my_gpu_script.py               # Run the Python script.
```

Explanation

- `#!/bin/bash`: This shebang line starts the script in the Bash shell.
- `#SBATCH`: These lines contain SLURM directives:
  - `--job-name`: Sets the name of the job.
  - `--partition`: Specifies the partition.
  - `--nodes`: Specifies the number of nodes.
  - `--ntasks-per-node`: Specifies the number of parallel tasks per node.
  - `--mem`: Memory required.
  - `--time`: Maximum time after which the job will be terminated.
  - `--output`: Filename for the job output.
- `module load`: Loads the necessary modules. Modules might include software, compilers, or libraries.
- `python my_gpu_script.py`: Executes the Python script using GPU.

Submitting a job

To submit the job to the cluster, use:

```
sbatch my_job.sh
```

After submitting, you can monitor the job status with `squeue`.

Interactive jobs

For debugging or testing, you might want to run commands interactively on a shell. You can request an interactive session with:

```
srun -N 1 -n 10 -p regular1 -t 01:00:00 --pty /bin/bash -i
```

Tips for effective computing

1. **Efficient use of resources**: Ensure that your code is optimized for parallel/GPU usage. Not all tasks are suitable, particularly those that are not highly parallelizable.
2. **Resource requests**: Request only the resources you need. Over-requesting leads to inefficiencies in cluster usage.
3. **Monitoring and profiling**: Regularly monitor and profile your jobs to understand their resource utilization and optimize accordingly.

🎉 That's all Folks!