*“The way the processor industry is going, is to add more and more cores, but nobody knows how to program those things. I mean, two, yeah; four, not really; eight, forget it”*

Steve Jobs, Apple CEO, 2008

# Lecture B.1.:
# Foundations of Parallel Computing

CS205: Computing Foundations for Computational Science
Dr. David Sondak
Spring Term 2021

HARVARD
School of Engineering
and Applied Sciences

IACS
INSTITUTE FOR APPLIED
COMPUTATIONAL SCIENCE
AT HARVARD UNIVERSITY

Lectures developed by Ignacio Illorente

# Before We Start

## Where We Are

Computing Foundations for Computational and Data Science

How to use modern computing platforms in solving scientific problems

Intro: Large-Scale Computational and Data Science

A. Parallel Processing Fundamentals

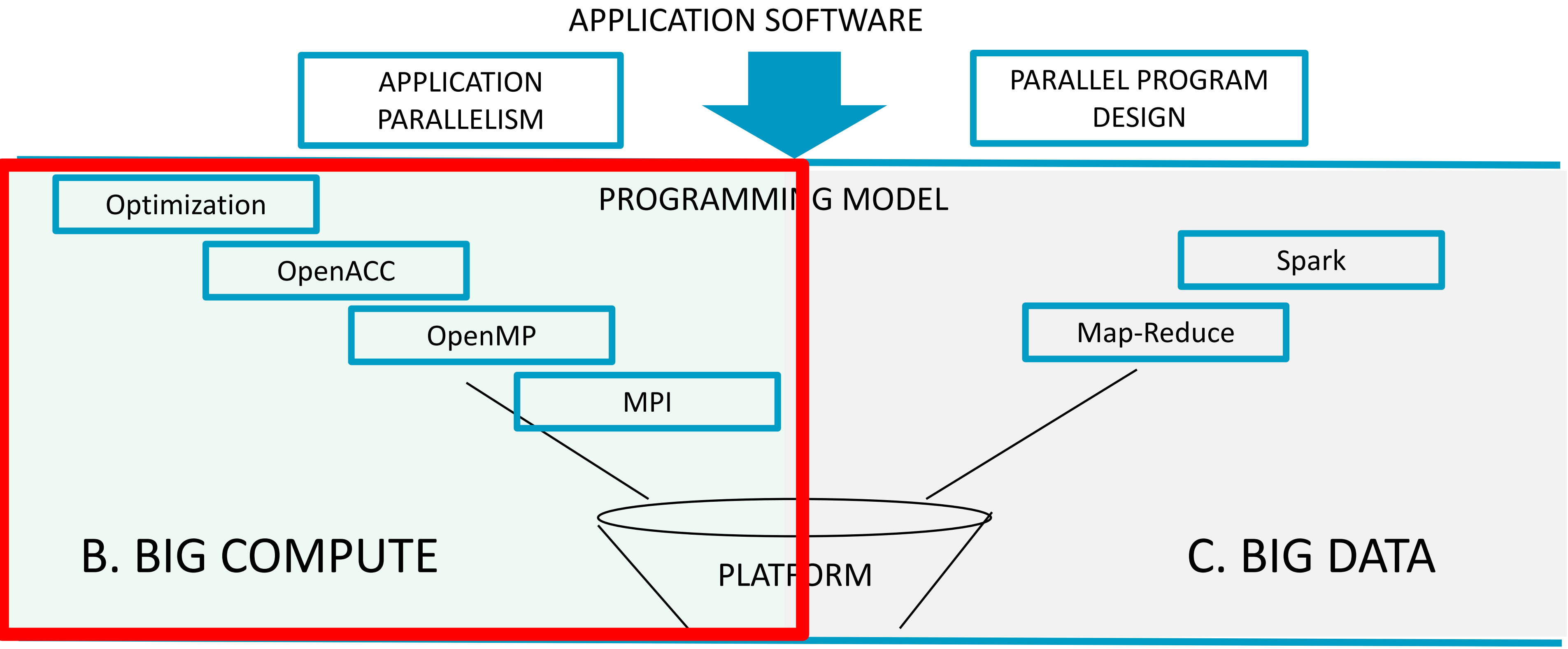
B. Parallel Computing

- B.1. Foundations of Parallel Computing
- B.2. Performance Optimization
- B.3. Accelerated Computing
- B.4. Shared-memory Parallel Processing
- B.5. Distributed-memory Parallel Processing

C. Parallel Data Processing

Wrap-Up: Advanced Topics

# CS205: Contents



APPLICATION SOFTWARE

APPLICATION PARALLELISM

PARALLEL PROGRAM DESIGN

PROGRAMMING MODEL

Optimization

OpenACC

OpenMP

MPI

Spark

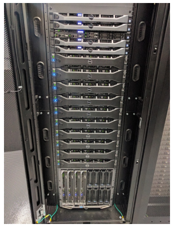
Map-Reduce

B. BIG COMPUTE

C. BIG DATA

PLATFORM

amazon web services



Open Nebula

FASRC

FASRC CANNON

HARVARD'S LARGEST CLUSTER

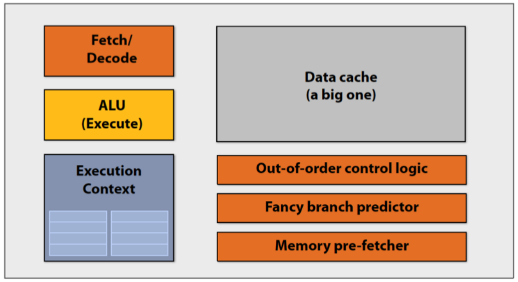
CLOUD COMPUTING

PARALLEL ARCHITECTURES

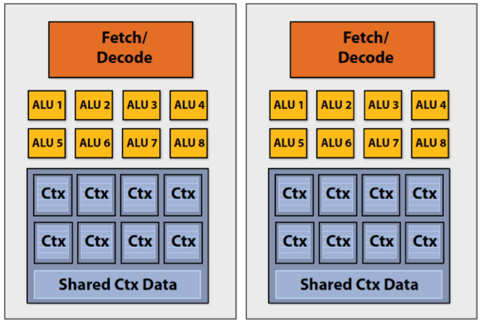
# Context

## Foundations of Parallel Computing

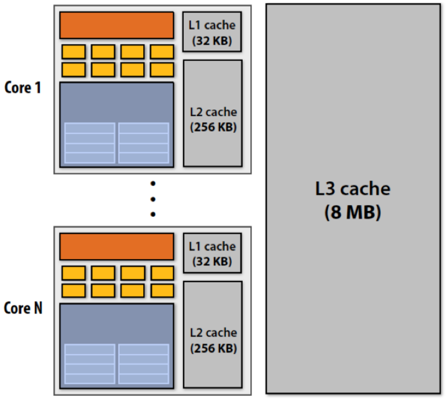
How to develop code that can make effective use of existing parallelism at different levels?



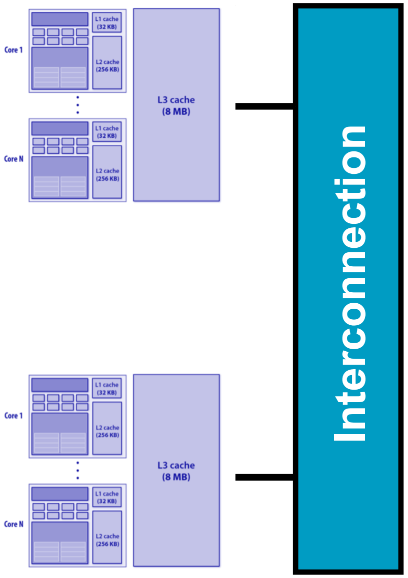
ILP/Data



Many-core



Multi-core



Multi-node

# Roadmap

## Foundations of Parallel Computing

Performance Optimization

Accelerated Computing

Shared-Memory Programming

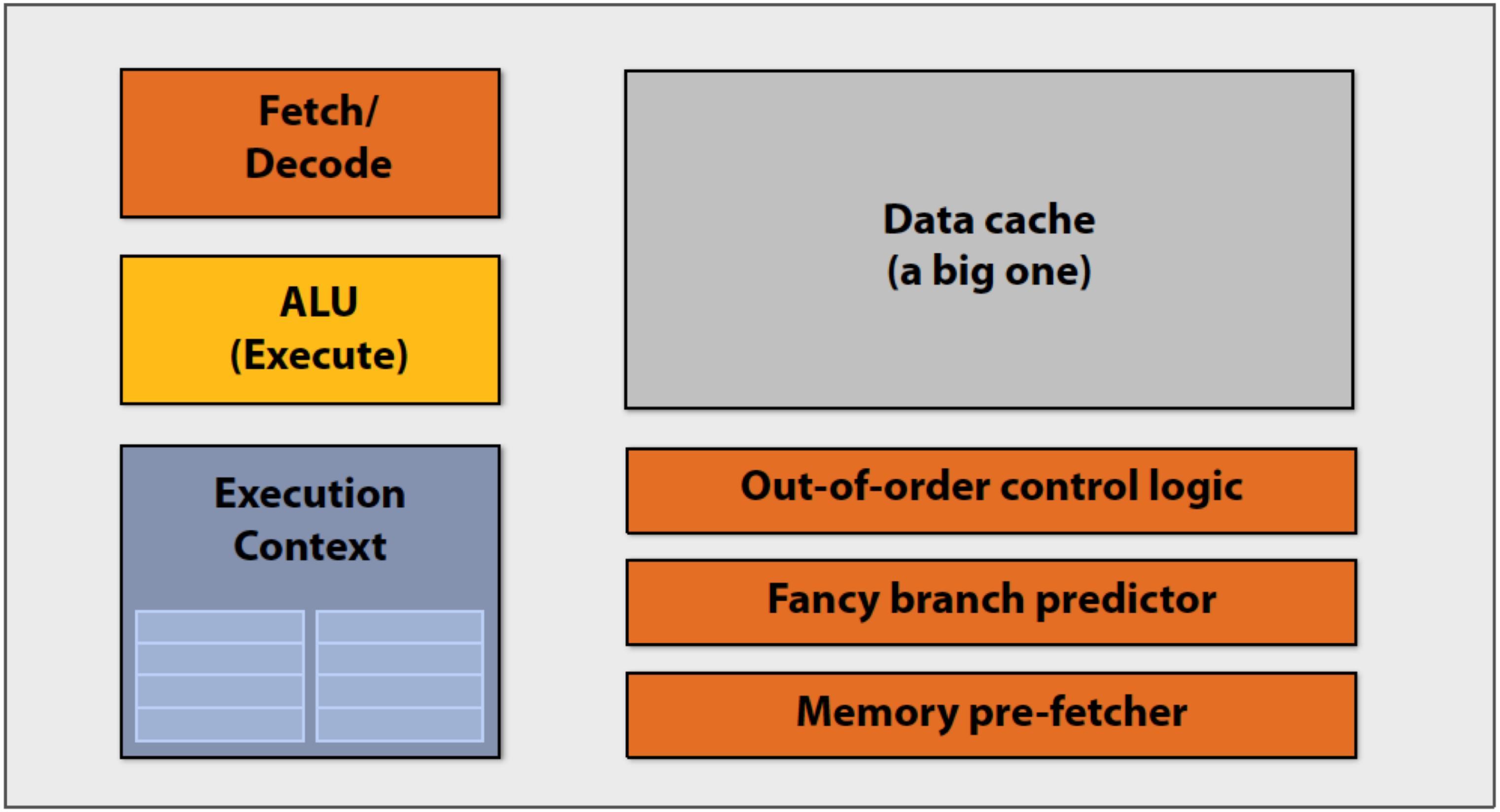
Distributed-Memory Programming

Reproducibility and Replicability

# PERFORMANCE OPTIMIZATION

# Performance Optimization

## Parallelism Level



# Performance Optimization

## Execution Model

CPUs Use Two Main Techniques for Performance

- Instruction Level Parallelism (Superscalar and Pipelining)
  - ✓ Superscalar processors have multiple “functional units” that can run in parallel
  - ✓ Pipelining is a form of parallelism, like an assembly line in a factory

- Caches (Memory Hierarchy)
  - ✓ Small amount of fast memory where values are “cached” in hope of reusing recently used or nearby data

# Performance Optimization

## Different Libraries and Approaches

Programmer/Compiler can adapt the code to exploit these two techniques

| Option | Level | Execution Time | Code Size | Memory Usage | Compile Time |
|---|---|---|---|---|---|
| -O0 | optimization for compilation time (default) | + | + | - | - |
| -O1 or -O | optimization for code size and execution time | - | - | + | + |
| -O2 | optimization more for code size and execution time | -- |  | + | ++ |
| -O3 | optimization more for code size and execution time | --- |  | + | +++ |
| -Os | optimization for code size |  | -- |  | ++ |
| -Ofast | O3 with fast none accurate math calculations | --- |  | + | +++ |

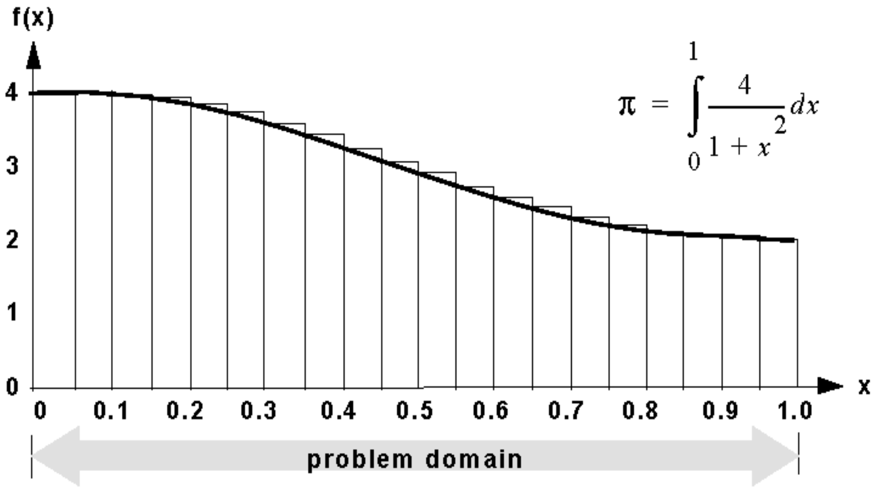
```
int x = 0;
for (i = 0; i < 101; i += 5) {
    x += 1;
    x += 1;
    x += 1;
    x += 1;
    x += 1;
}
```

# Performance Optimization

## Anatomy of an Application

### An Example: Pi with Loop Unrolling

```
#include <stdio.h>
#define N 2000000000
#define vl 1024
int main(void) {
  double pi = 0.0f;
  long long i;
  for (i=0; i<N; i++) {
    double t= (double)((i+0.5)/N);
    pi +=4.0/(1.0+t*t);
}
  printf("pi=%11.10f\n",pi/N);
  return 0;
}
```



# Performance Optimization

## Anatomy of an Application

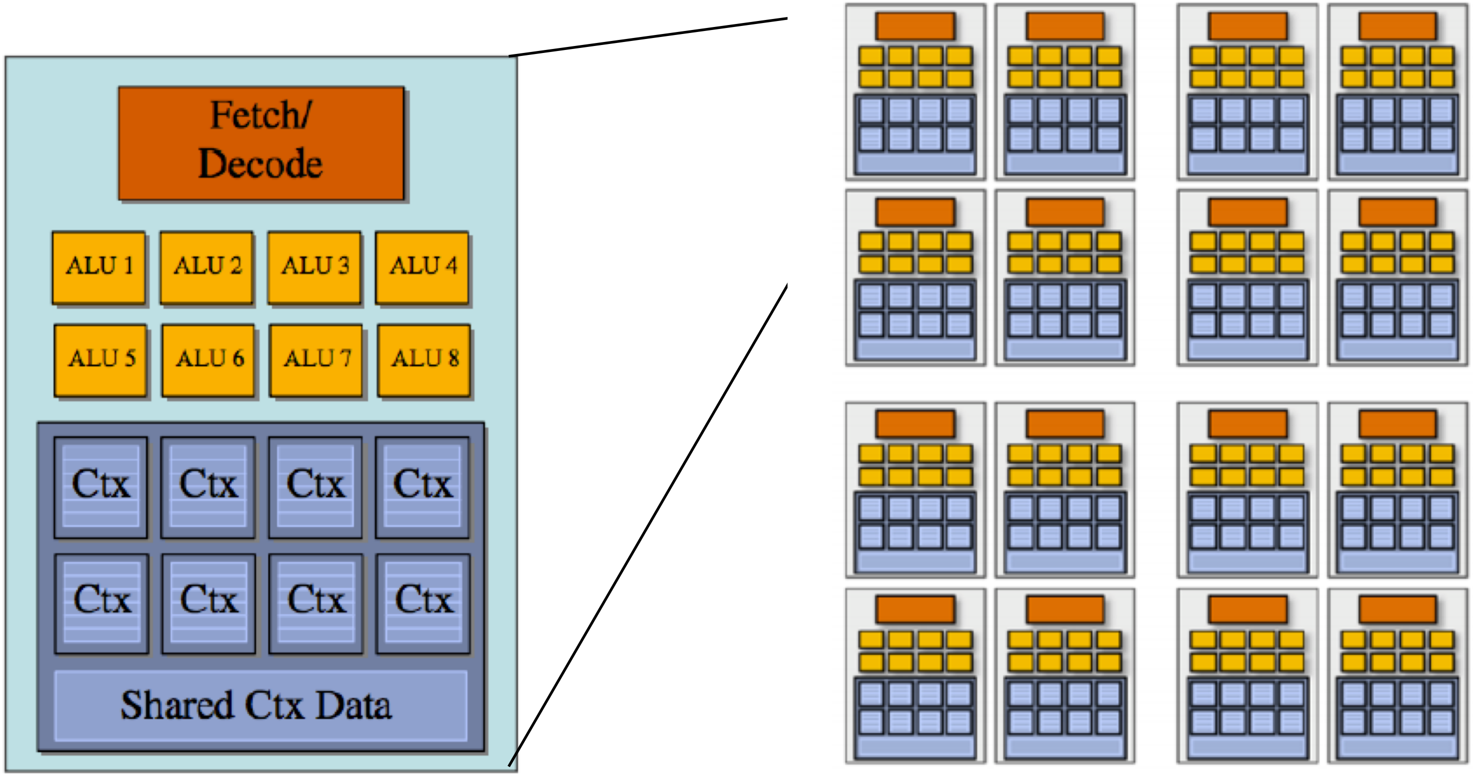
### An Example: Pi with Loop Unrolling

```c
#include <stdio.h>
#define N 2000000000
#define vl 1024
int main(void) {
  double pi = 0.0f;
  long long i;
  for (i=0; i<N; i+=2) {
    double t= (double)((i+0.5)/N);
    pi +=4.0/(1.0+t*t);
    t= (double)((i+1+0.5)/N);
    pi +=4.0/(1.0+t*t);
  }
  printf("pi=%11.10f\n",pi/N);
  return 0;
}
```

# ACCELERATED COMPUTING

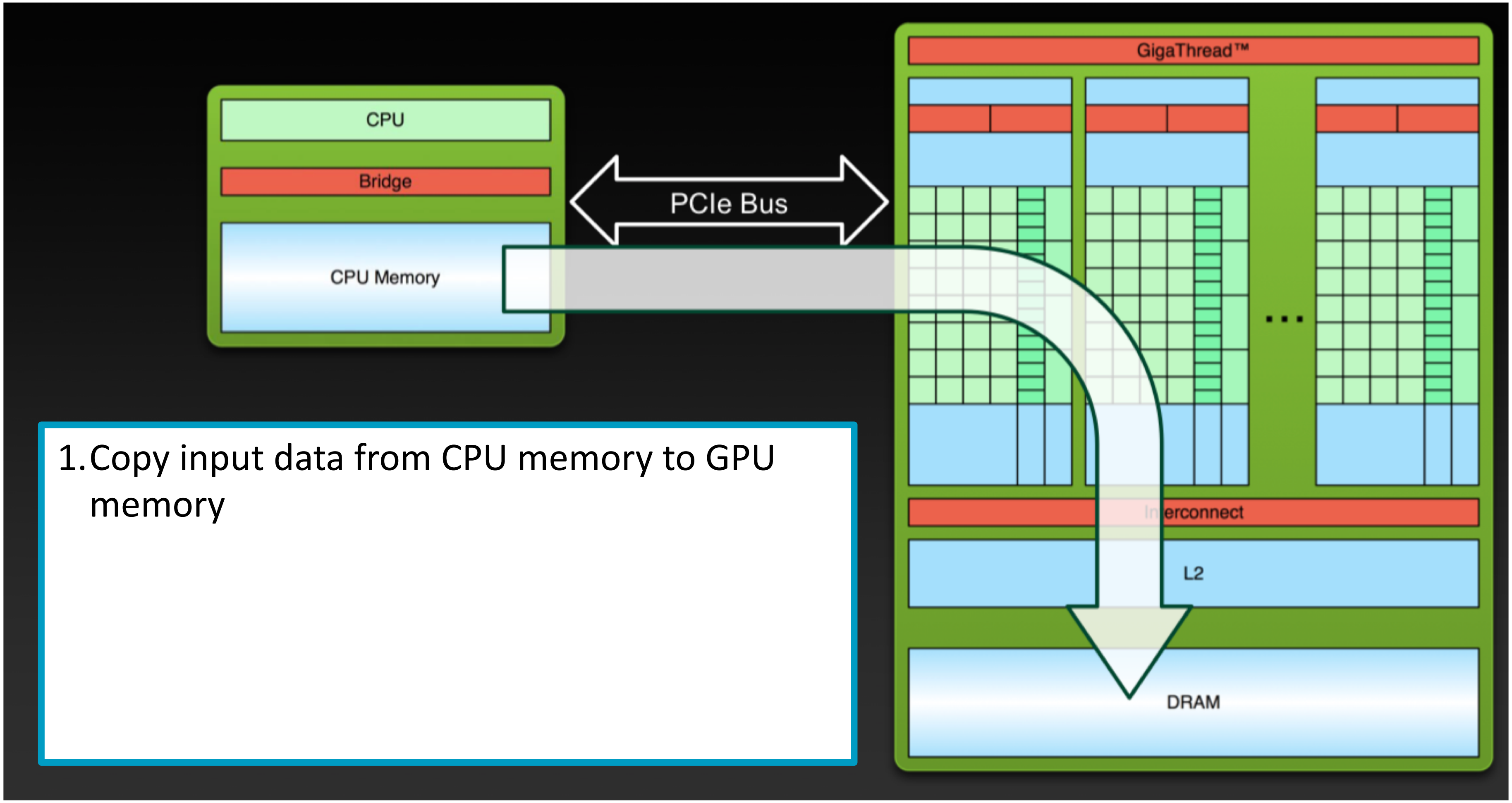
# Accelerated Computing

## Parallelism Level



# Accelerated Computing

## Execution Model

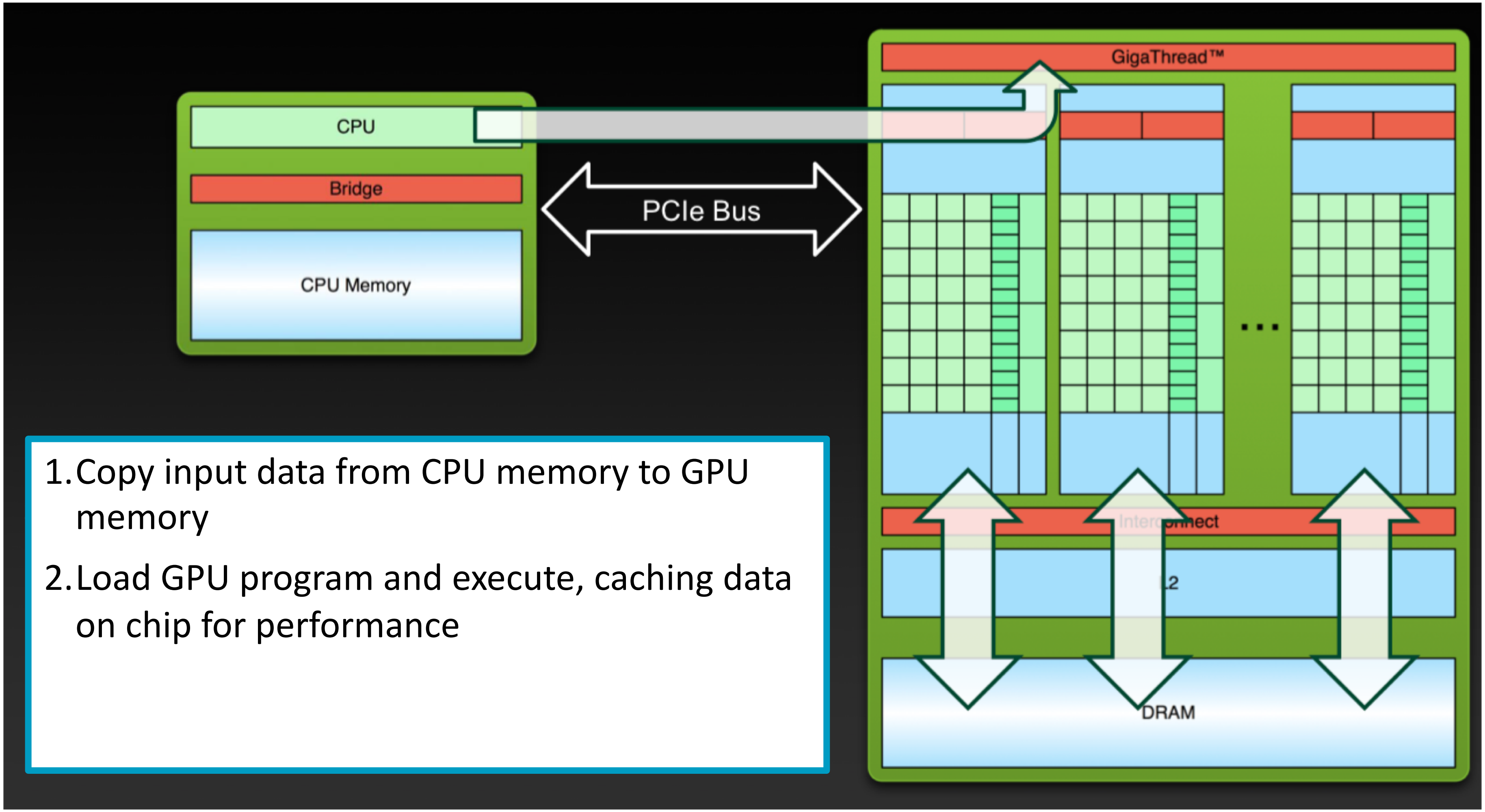


1. Copy input data from CPU memory to GPU memory

Source: NVIDIA

# Accelerated Computing

## Execution Model

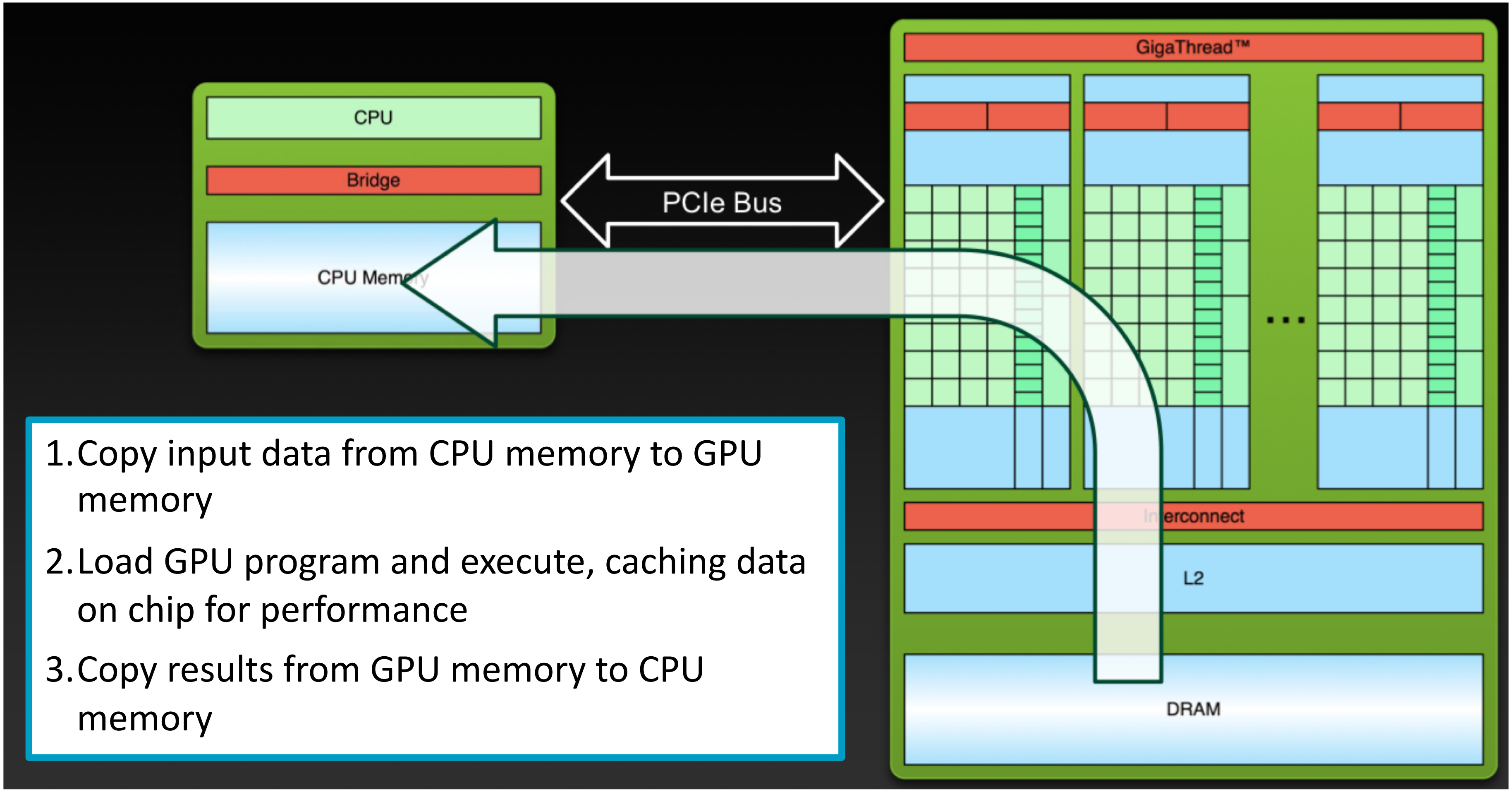


1. Copy input data from CPU memory to GPU memory
2. Load GPU program and execute, caching data on chip for performance

Source: NVIDIA

# Accelerated Computing

## Execution Model

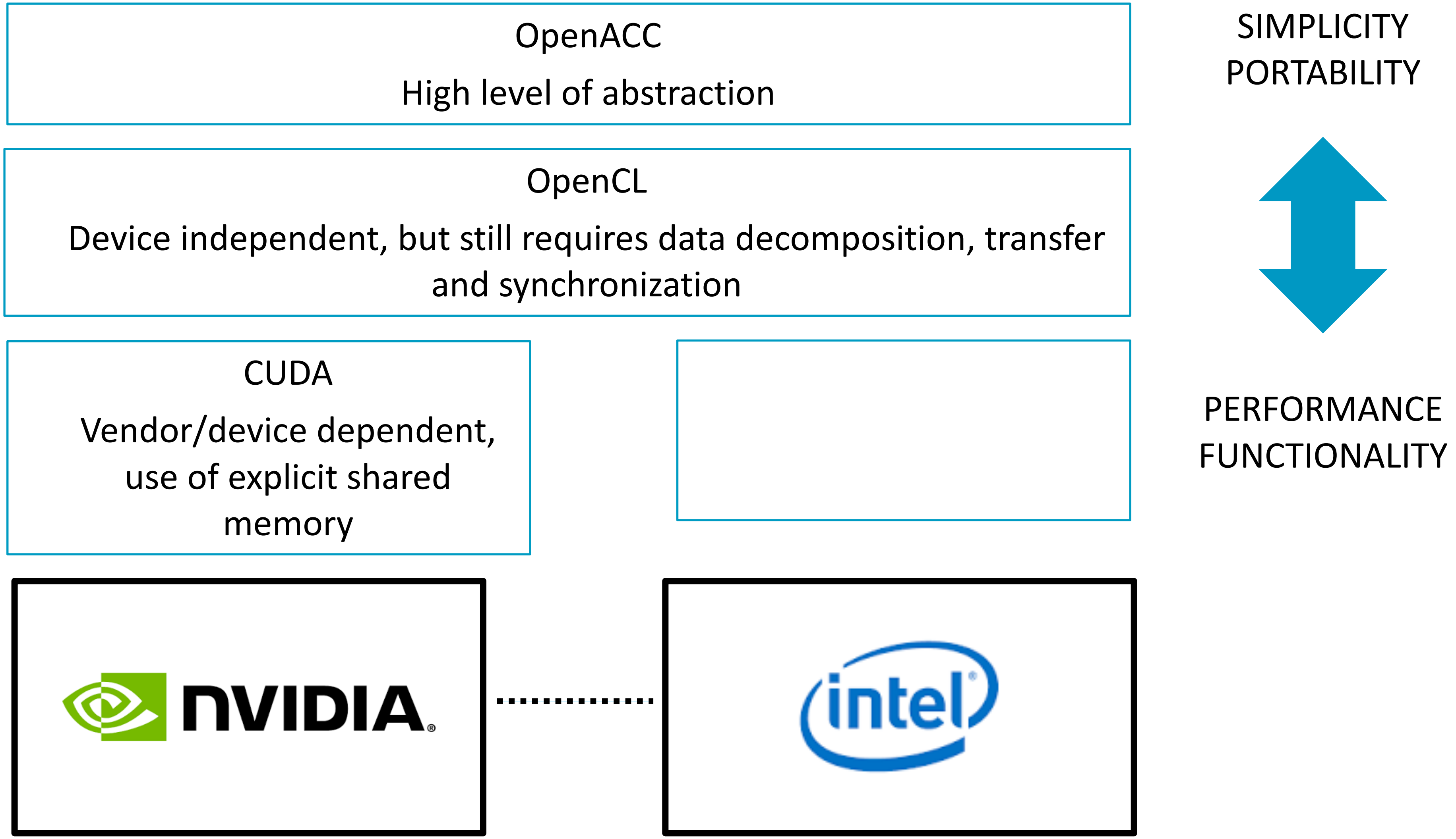


1. Copy input data from CPU memory to GPU memory
2. Load GPU program and execute, caching data on chip for performance
3. Copy results from GPU memory to CPU memory

Source: NVIDIA

# Accelerated Computing

## Different Libraries and Approaches



**OpenACC**

High level of abstraction

**OpenCL**

Device independent, but still requires data decomposition, transfer and synchronization

**CUDA**

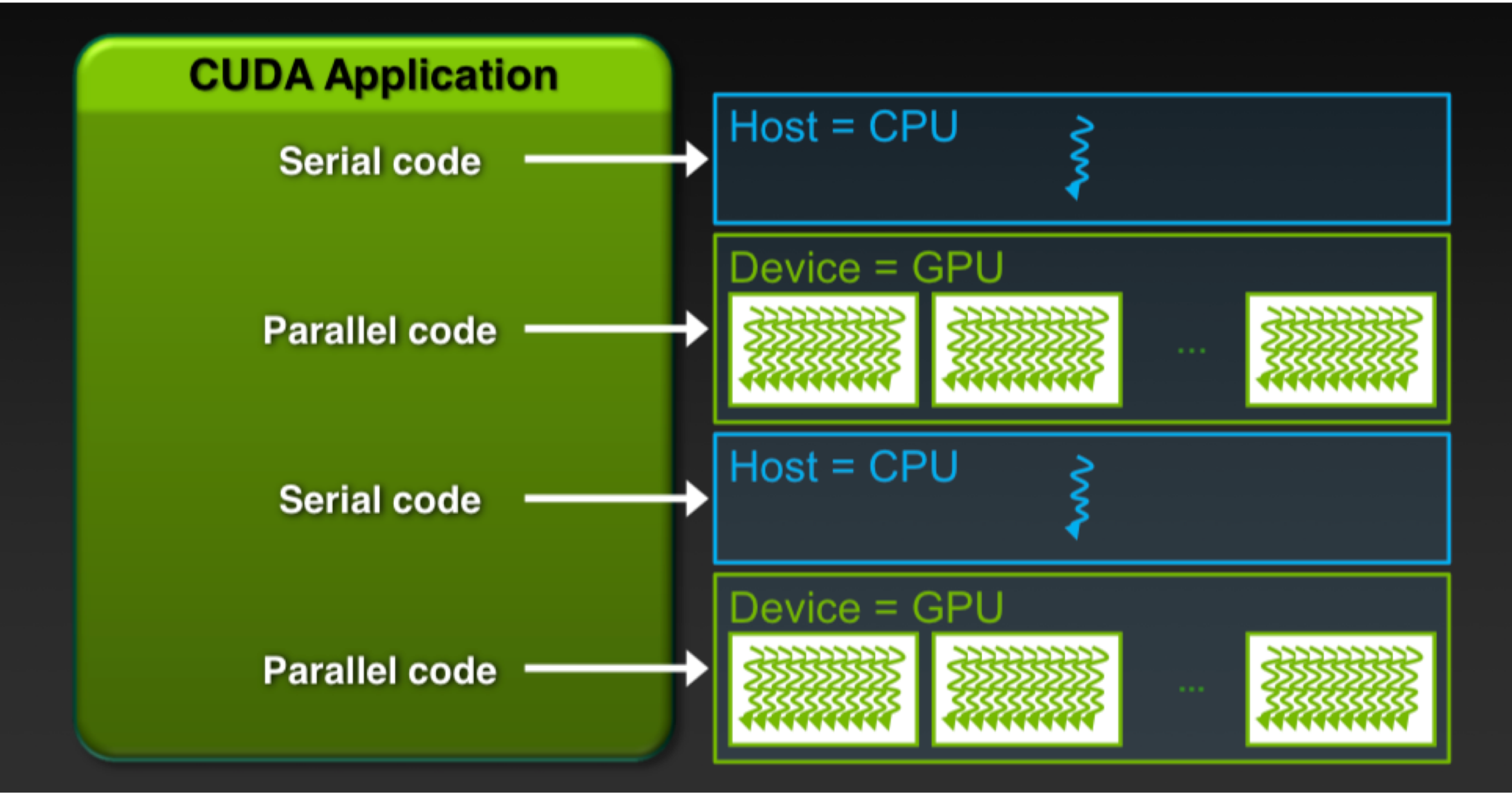
Vendor/device dependent, use of explicit shared memory

SIMPLICITY
PORTABILITY

PERFORMANCE
FUNCTIONALITY

# Accelerated Computing

## Anatomy of an Application



Source: NVIDIA

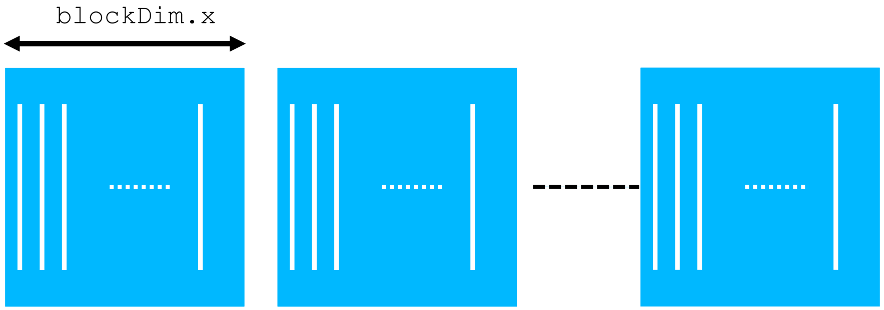
# Accelerated Computing

## Anatomy of an Application

**CUDA**

### An Example: SAXPY with CUDA

```
#include <stdio.h>

__global__
void saxpy(int n, float a, float *x, float *y)
{
  int i = blockIdx.x*blockDim.x + threadIdx.x;
  if (i < n) y[i] = a*x[i] + y[i];
}

int main(void)
{
  int N = 1<<20;
  float *x, *y, *d_x, *d_y;
  x = (float*)malloc(N*sizeof(float));
  y = (float*)malloc(N*sizeof(float));

  cudaMalloc(&d_x, N*sizeof(float));
  cudaMalloc(&d_y, N*sizeof(float));

  for (int i = 0; i < N; i++) {
    x[i] = 1.0f;
    y[i] = 2.0f;
  }

  cudaMemcpy(d_x, x, N*sizeof(float), cudaMemcpyHostToDevice);
  cudaMemcpy(d_y, y, N*sizeof(float), cudaMemcpyHostToDevice);

  // Perform SAXPY on 1M elements
  saxpy<<<(N+255)/256, 256>>>(N, 2.0f, d_x, d_y);

  cudaMemcpy(y, d_y, N*sizeof(float), cudaMemcpyDeviceToHost);
 …
}
```



# Accelerated Computing

## Anatomy of an Application

**OpenACC**

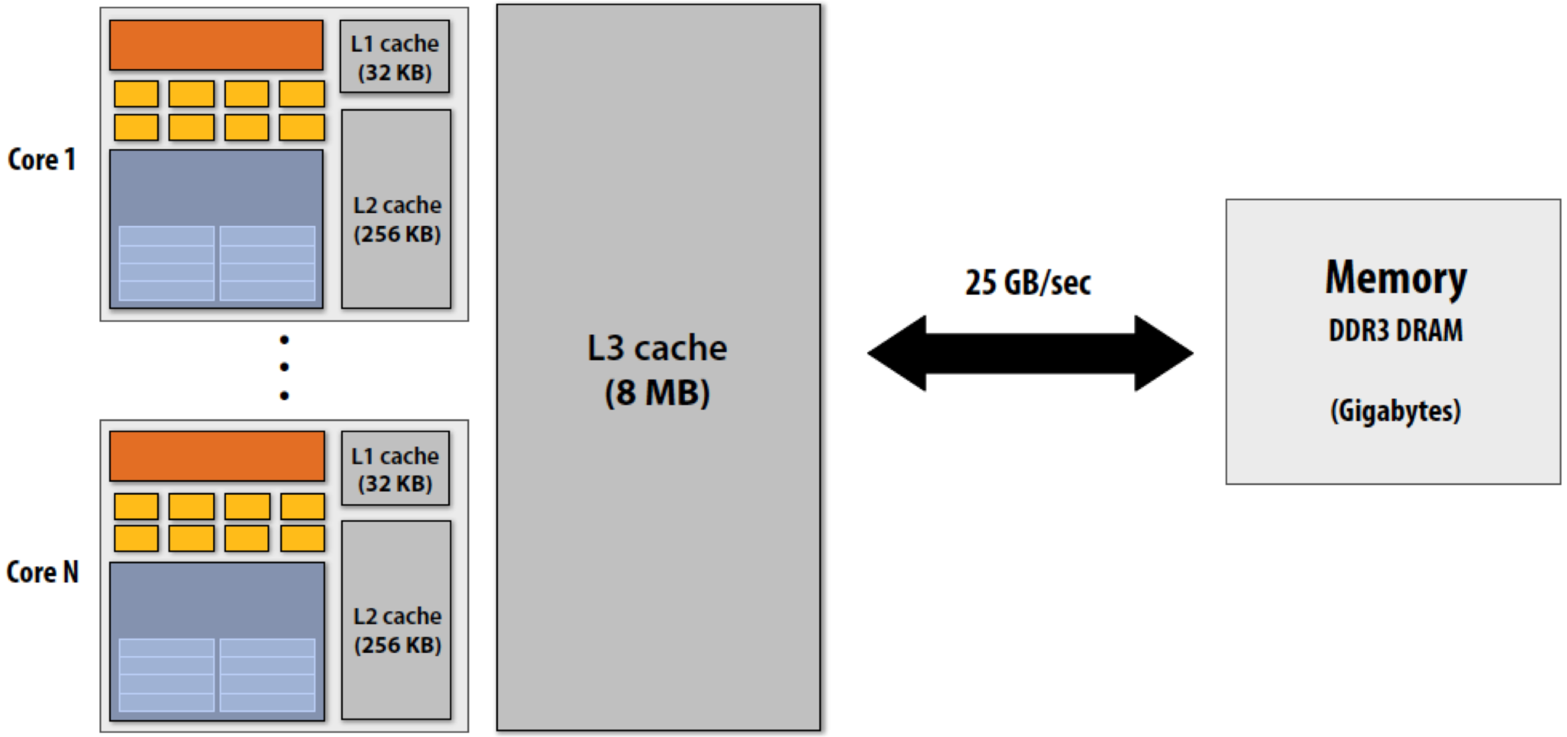
An Example: Pi with OpenACC

```
#include <stdio.h>
#define N 2000000000
#define vl 1024
int main(void) {
  double pi = 0.0f;
  long long i;
  #pragma acc parallel vector_length(vl)
  #pragma acc loop reduction(+:pi)
  for (i=0; i<N; i++) {
    double t= (double)((i+0.5)/N);
    pi +=4.0/(1.0+t*t);
  }
  printf("pi=%11.10f\n",pi/N);
  return 0;
}
```

# SHARED-MEMORY PROGRAMMING

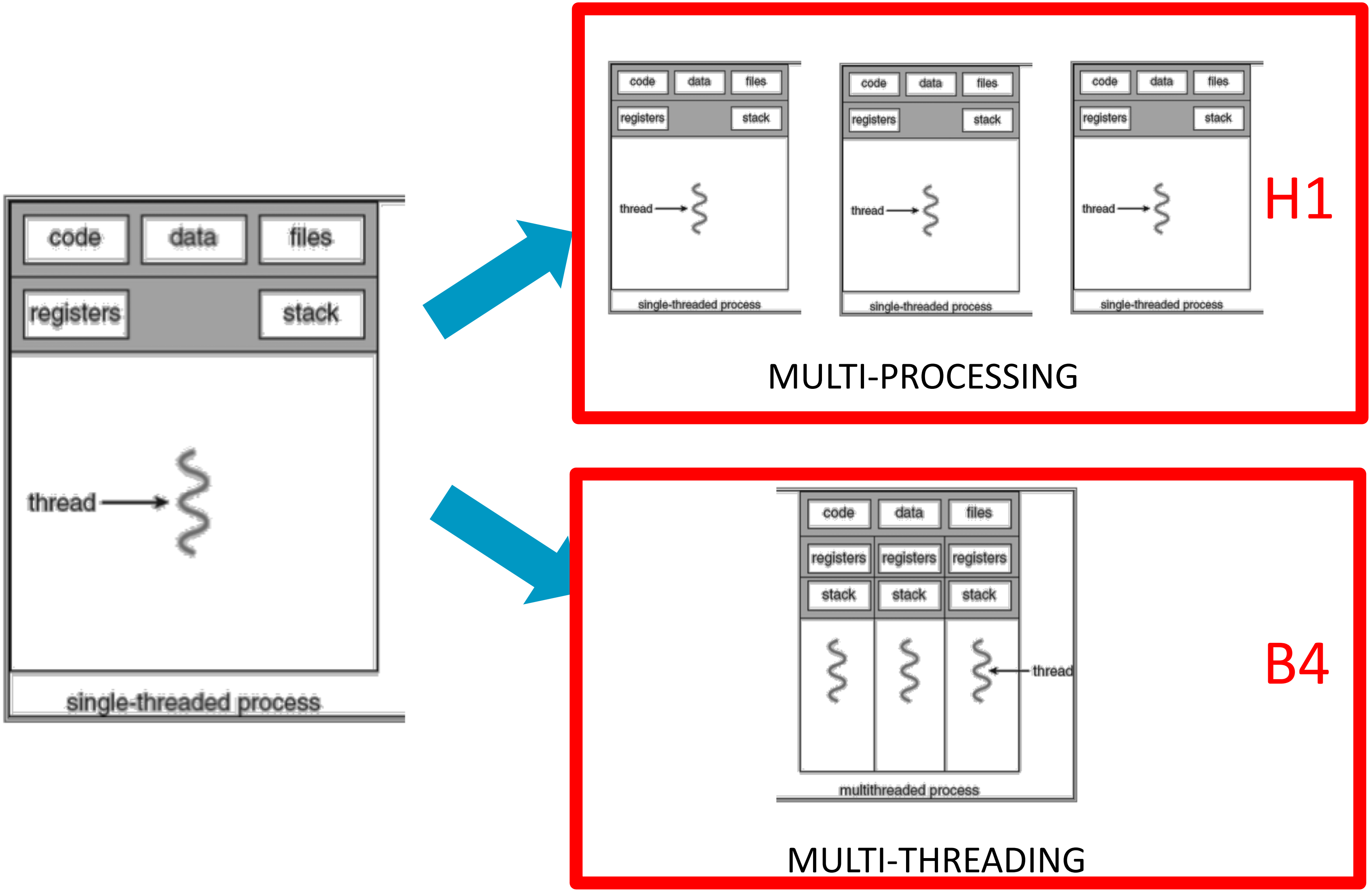
# Shared-Memory Programming

## Parallelism Level



# Shared-Memory Programming

## Execution Model



H1

MULTI-PROCESSING

B4

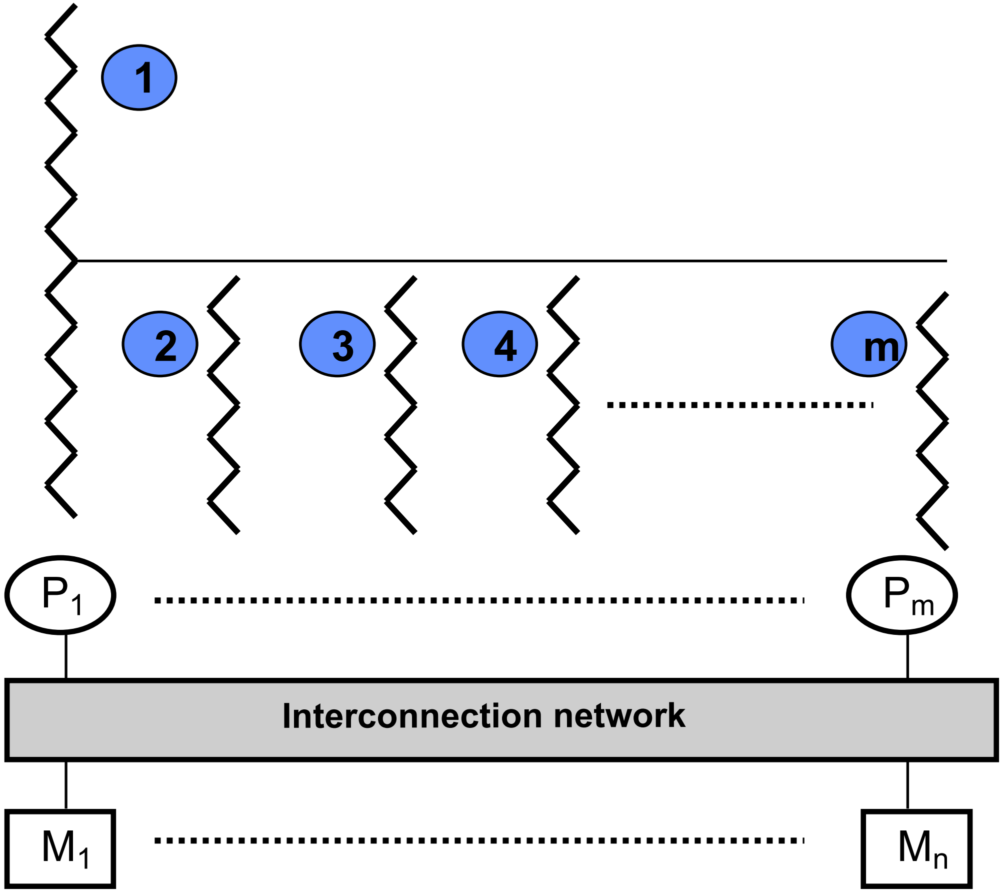
MULTI-THREADING

# Shared-Memory Programming

## Execution Model

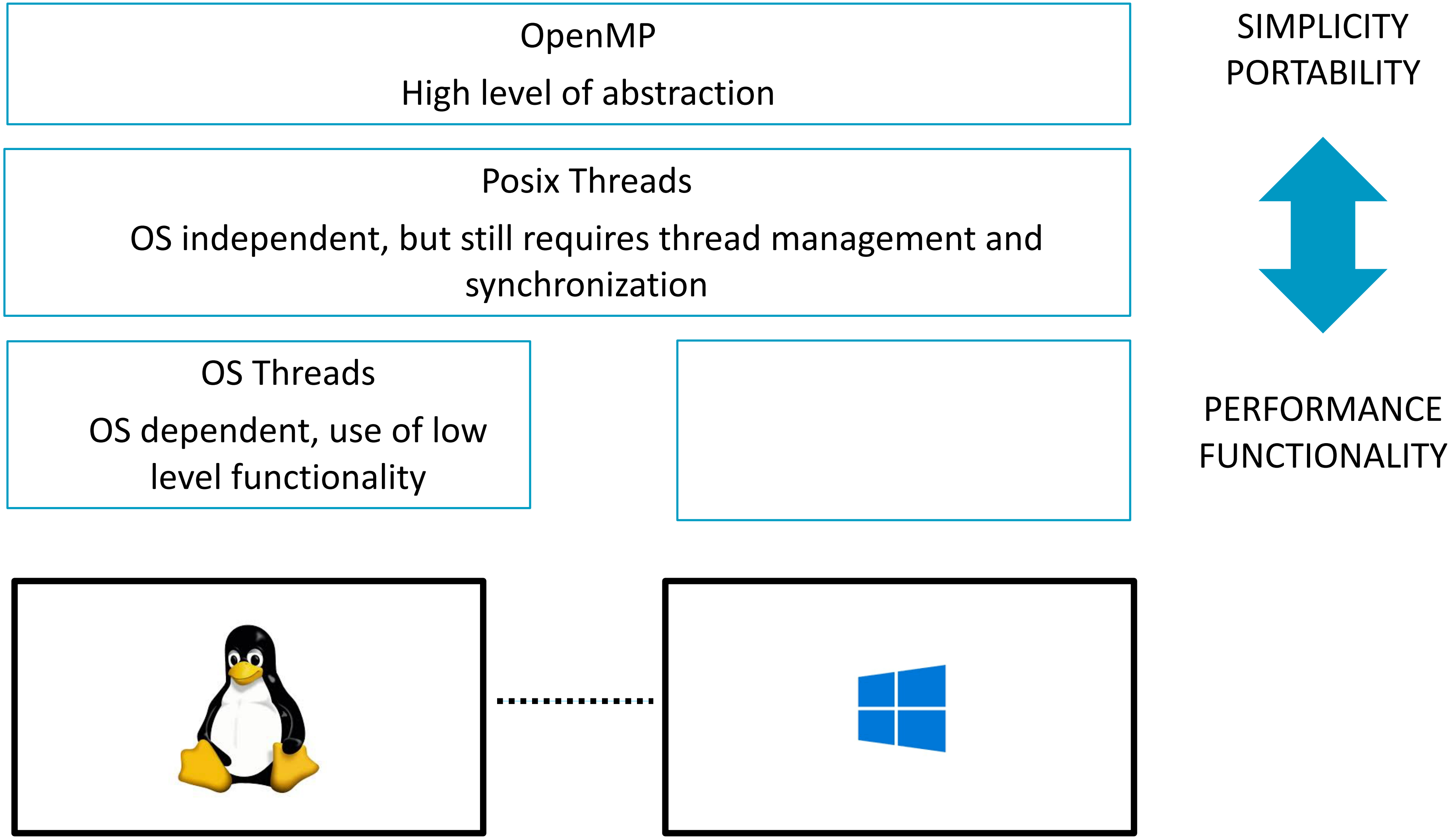
**Description**

- Shared memory communication
- Thread management routines
  - Create
  - Wait
  - Synchronization
  - …



# Shared-Memory Programming

## Different Libraries and Approaches



OpenMP

High level of abstraction

Posix Threads

OS independent, but still requires thread management and synchronization

OS Threads

OS dependent, use of low level functionality

SIMPLICITY
PORTABILITY

PERFORMANCE
FUNCTIONALITY

# Shared-Memory Programming

## Anatomy of an Application

**Posix Threads**

### An Example: Hello World

```
void *print_message_function( void *ptr );
pthread_mutex_t mutex;
main()
{
     pthread_t thread1, thread2;
     pthread_attr_t pthread_attr_default;
     pthread_mutexattr_t pthread_mutexattr_defa
     struct timespec delay;
     char *message1 = "Hello";
     char *message2 = "World\n";

     delay.tv_sec = 10;
     delay.tv_nsec = 0;

     pthread_attr_init(&pthread_attr_default);
     pthread_mutexattr_init(&pthread_mutexattr_default);

     pthread_mutex_init(&mutex, &pthread_mutexattr_default);
     pthread_mutex_lock(&mutex);

     pthread_create( &thread1, &pthread_attr_default,
                     (void *) print_message_function, (void *) message1);
     pthread_mutex_lock(&mutex);
     pthread_create(&thread2, &pthread_attr_default,
                     (void *) print_message_function, (void *) message2);
     pthread_mutex_lock(&mutex);
     exit(0);
}
```

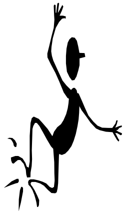
```
void *print_message_function( void *ptr )
{
     char *message;
     message = (char *) ptr;
     printf("%s ", message);
     pthread_mutex_unlock(&mutex);
     pthread_exit(0);
}
```

# Shared-Memory Programming

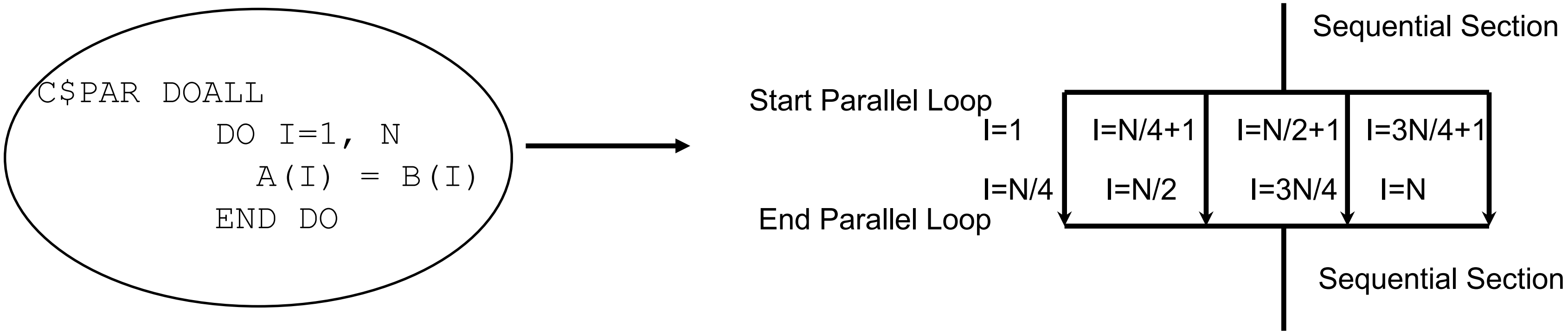
## Different Libraries and Approaches

### Easy Multi-threading Programming with Directives

**Thread programming problems**
- Management of too many threads
- Data Races, Deadlocks, and Live Locks



**Parallelization Directives**
- Execute loop on multiple cores



```
C$PAR DOALL
        DO I=1, N
          A(I) = B(I)
        END DO
```

Sequential Section

Start Parallel Loop

| I=1 | I=N/4+1 | I=N/2+1 | I=3N/4+1 |
|---|---|---|---|
| I=N/4 | I=N/2 | I=3N/4 | I=N |

End Parallel Loop

Sequential Section

**Higher-level Abstraction**
- Faster development and more portable
- But not so flexible and efficient

# Shared-Memory Programming

## Anatomy of an Application

**OpenMP**

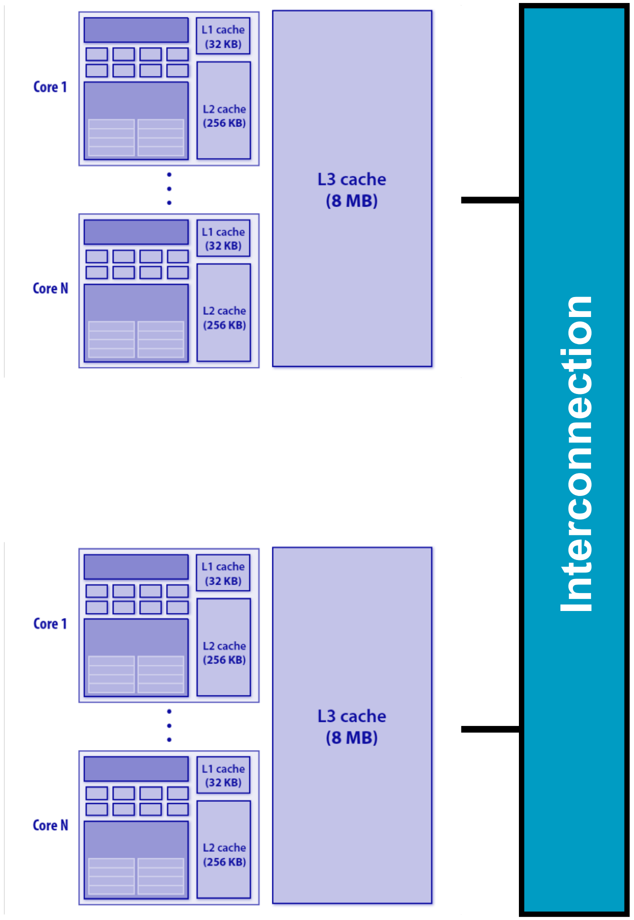
An Example: Hello World

```
#include <stdio.h>
#define N 2000000000
#define vl 1024
int main(void) {
  double pi = 0.0f;
  long long i;
  #pragma omp parallel for reduction(+:pi) private(i,t)
  for (i=0; i<N; i++) {
    double t= (double)((i+0.5)/N);
    pi +=4.0/(1.0+t*t);
  }
  printf("pi=%11.10f\n",pi/N);
  return 0;
}
```

# DISTRIBUTED-MEMORY COMPUTING

# Distributed-Memory Programming

## Parallelism Level

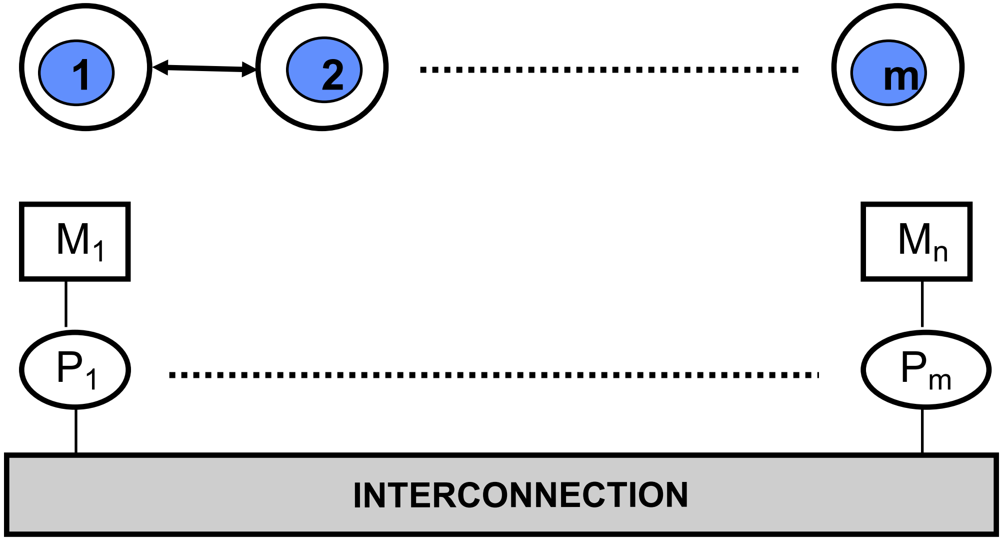


# Distributed-Memory Programming

## Execution Model

**Description**

- Message passing communication
- Communication management routines
  - Send
  - Receive
  - Synchronization
  - …



# Distributed-Memory Programming

## Anatomy of an Application

### MPI (*Message Passing Interface*)

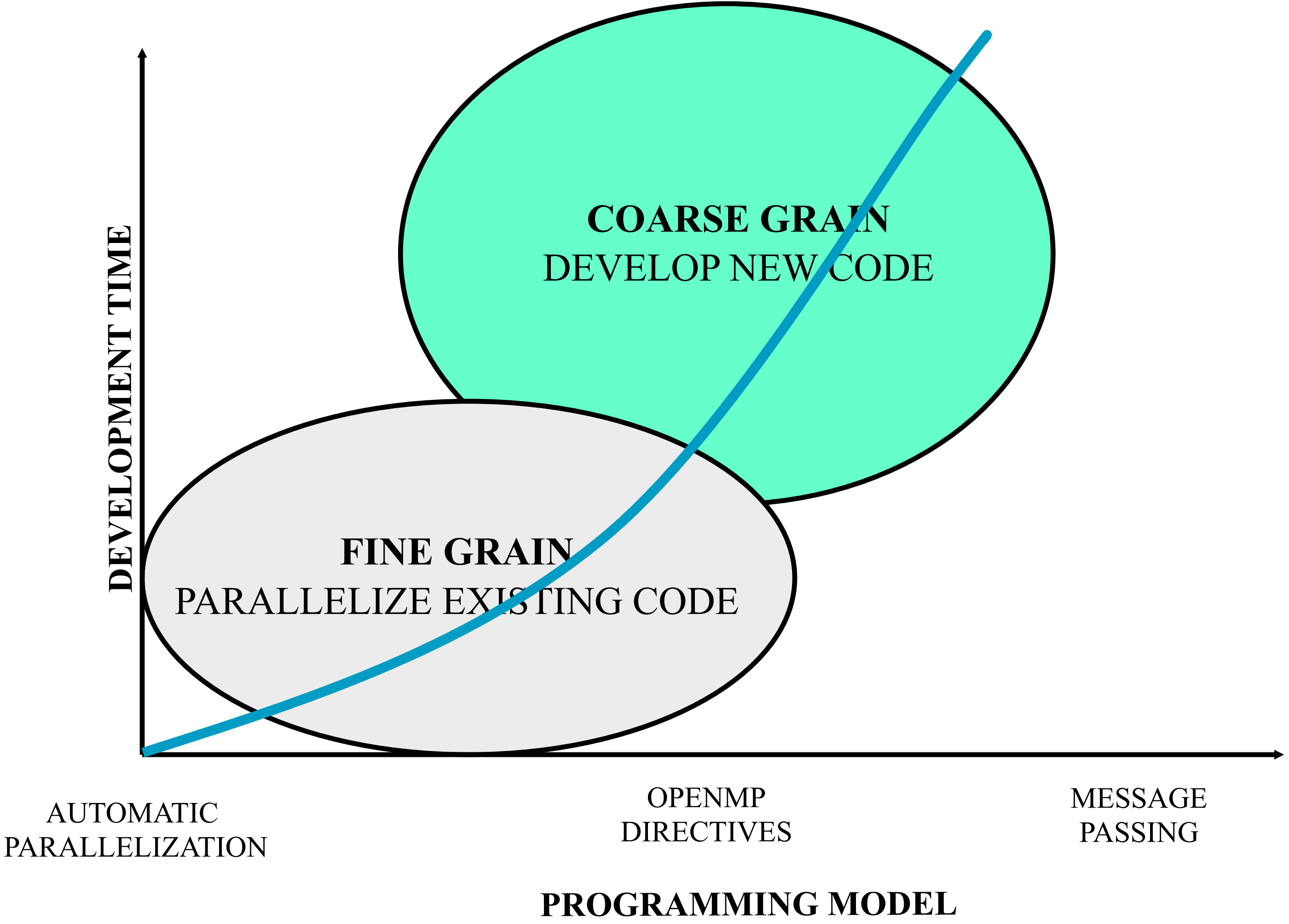
Basic Program Structure (Only 6 routines)

```
#include <stdio.h>
#include <mpi.h>

main(int argc, char **argv)
  {
    int rank, size, tag=50, destination=0, source;
    char message[100];
    MPI_Status state;
    MPI_Init(&argc, &argv);
    MPI_Comm_rank(MPI_COMM_WORLD, &rank);
    MPI_Comm_size(MPI_COMM_WORLD, &size);

    if (rank !=0) {
      sprintf(message,"¡Greetings from process %d!", rank);
      MPI_Send(message, strlen(message)+1, MPI_CHAR, destination, tag, MPI_COMM_WORLD);
    } else {
      for (source = 1; source < size; source++) {
        MPI_Recv(message, strlen(message)+1, MPI_CHAR, source, tag, MPI_COMM_WORLD, &state);
        printf("%s\n", message);
      }
    }
    MPI_Finalize();
  }
```

# Distributed-Memory Programming

## Shared vs Distributed Memory

### The Right Model Depends on (Time, Cost, Performance)



# Reproducibility and Replicability

## The Four Rs

**Reusability**

- Reusability refers to the possibility to reuse the software or parts of it for different purposes, in different environments, and by researchers other than the original authors.

**Rewriteability**

- Rewriteability refers to the possibility to modify and extend the software or parts of it.

**Reproducibility**

- Reproducibility of a computational experiment means that it can be repeated by a different researcher in a different computing infrastructure but with the same execution environment and to come to the same numerical results.

**Replicability**

- The attribute Replicability describes the ability to repeat a computational experiment on the same computing infrastructure and to come to the same numerical results and computing performance.

# Reproducibility and Replicability

## The Four Rs

AERODYNAMICS

NAVIER-STOKES

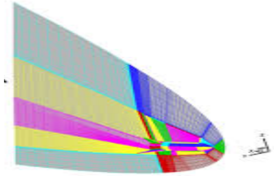
$$\frac{\partial u}{\partial t}+\frac{1}{r^\tau}\frac{\partial(r^\tau uu)}{\partial r}+\frac{\partial(vu)}{\partial z}=-\frac{\partial p}{\partial r}+\frac{1}{Re}\frac{\partial}{\partial z}\left(\frac{\partial u}{\partial z}-\frac{\partial v}{\partial r}\right)+\frac{1}{Fr^2}g_r,$$

$$\frac{\partial v}{\partial t}+\frac{1}{r^\tau}\frac{\partial(r^\tau uv)}{\partial r}+\frac{\partial(vv)}{\partial z}=-\frac{\partial p}{\partial z}+\frac{1}{Re\,r^\tau}\frac{\partial}{\partial r}\left(r^\tau\left(\frac{\partial u}{\partial z}-\frac{\partial v}{\partial r}\right)\right)+\frac{1}{Fr^2}g_z,$$

$$\frac{1}{r^\tau}\frac{\partial(r^\tau u)}{\partial r}+\frac{\partial v}{\partial z}=0,$$

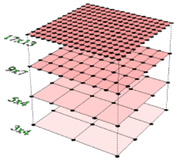
PHYSICS

FINITE DIFFERENCE



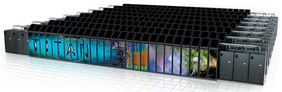
ACCURACY

MULTIGRID



COMPLEXITY

PARALLEL



SPEED-UP

### EXECUTION ENVIRONMENT

- Algorithm, application version and dependencies

- VIRTUAL MACHINES
- SOFTWARE CONTAINERS

### SYSTEM CAPACITY

- Execution time, performance…

- CLOUD PROVIDERS

# Reproducibility and Replicability

## Different Results for the Same Program?

### NON-REPRODUCIBLE BEHAVIORS

- A bug in the software or a fault in the hardware
- Floating-point numbers cannot precisely represent all real numbers bringing rounding and overflow errors
- Code and compiler options may change operation ordering, sometimes x=a+b+… differs from x=b+a… (non-commutativity)
- Parallel processing changes operation ordering, sometimes, x=a+b+c+d does not give the same results when computed (on two units) either as x=(a+b)+(c+d) or x=(a+c)+(b+d) (non-associativity).

# Reproducibility and Replicability

## Round-off Error Propagation

### NUMERICAL ACCURACY OF REDUCTION OPERATIONS

Floating point representation of real numbers may bring two types of error:

- **Overflow:** Representation range limited by the exponent
- **Round-off:** Finite number of bits in mantissa

**IEEE 754**: 53 bits mantissa / 11 bits exponent

2**1023 = 8.9 10^307; 2**1024 = Inf

1.0 +2**(-53) = 1

- **Error Accumulation**
- **Catastrophic Cancellation**

(-100.0+100.0+1.0e-15)*1.0e+32 = 1.0e+17

(-100.0+ 1.0e-15+100.0)*1.0e+32 = 0.0

# Next Steps

- **Lab session** this week:
    - I2. OpenNebula Private Cloud Sandbox on AWS
    - I3. Docker on AWS

- Get ready for first **hands-on:**
    - H1. Python Multiprocessing

# Questions

## Foundations of Parallel Computing