High Performance Computing for Science and Engineering II

1.4.2019 - **Lecture 7: PGAS Model / UPC++**

Lecturer: Dr. Sergio Martin

Contains Slides from:
"UPC++: A PGAS Library for Exascale Computing"
By Scott B. Baden (Berkeley Lab). Used with permission.

CSElab
Computational Science & Engineering Laboratory

ETH zürich

Today's Class

High Throughput vs High Performance:

- Rationale and Examples

Sampling Engines & Tasking Strategies

- Divide-and-Conquer, Producer-Consumer

Message Passing Model

- Review & Limitations

PGAS Model

- UPC++, rationale and examples.

General Info

Grading Review and Feedback

- Moodle: Short statement, just for coarse-grained feedback
- More info: Send your grader an email
- In-depth review: Arrange a meeting with your grader

Homework 4

- Deadline in 3 Weeks
- Will contain bonus items -> +0.25 to any HW if done right

Next Week (8/4)

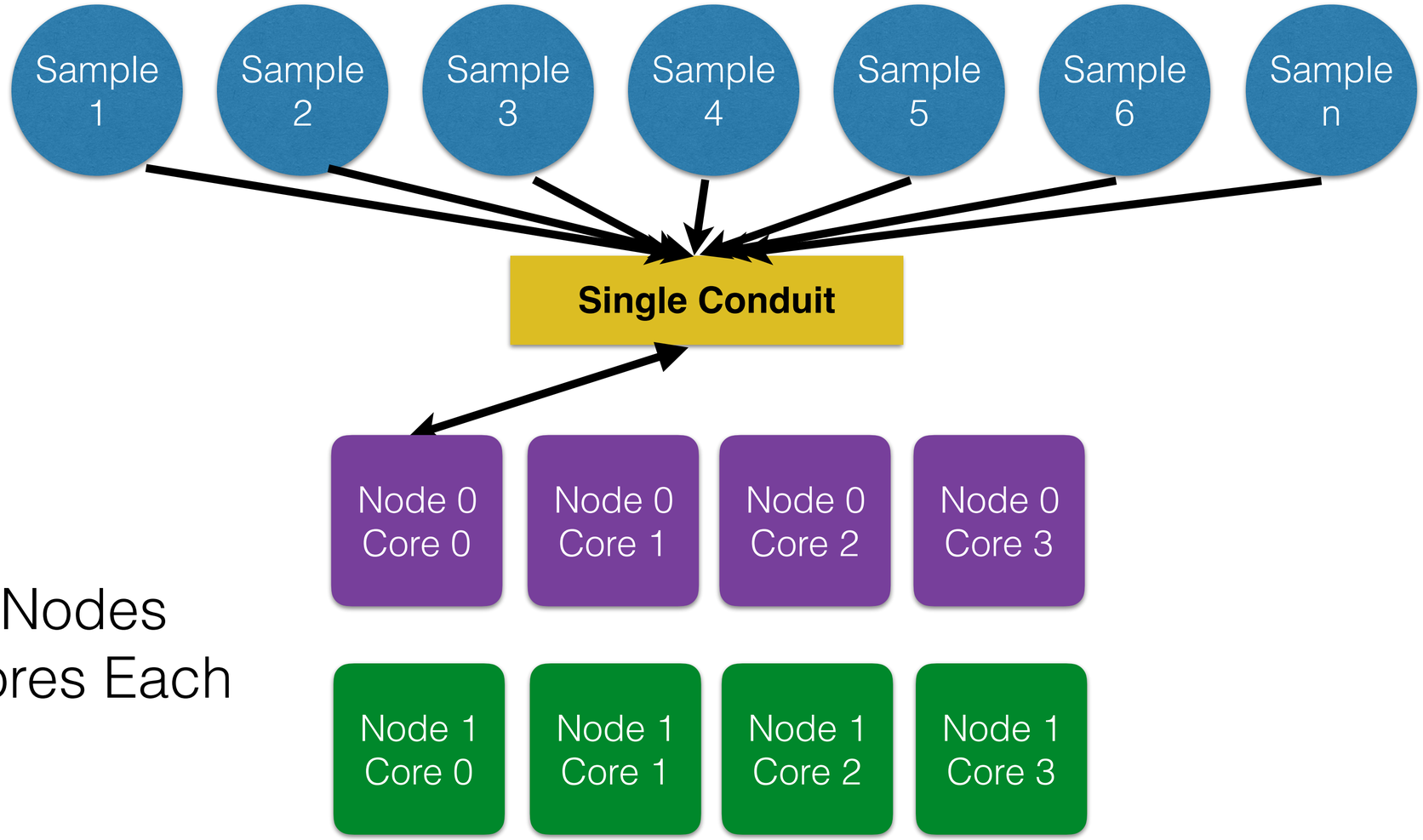
- There will be practice session -> UPC++ Practice
- There will be NO lecture.

Remember to get your Piz Daint Account!

High Throughput
vs
High Performance

Single-Core Conduit

Sample Population (Generation 0)



2 Nodes
4 Cores Each

Single-Core Conduit & Single-Core Model

Single-Core Sampler Conduit - Single-Core Model

Node 0 Core 0

Node 0 Core 1

Node 0 Core 2

Node 0 Core 3

Node 1 Core 0

Node 1 Core 1

Node 1 Core 2

Node 1 Core 3

Sample 0

Sample 1

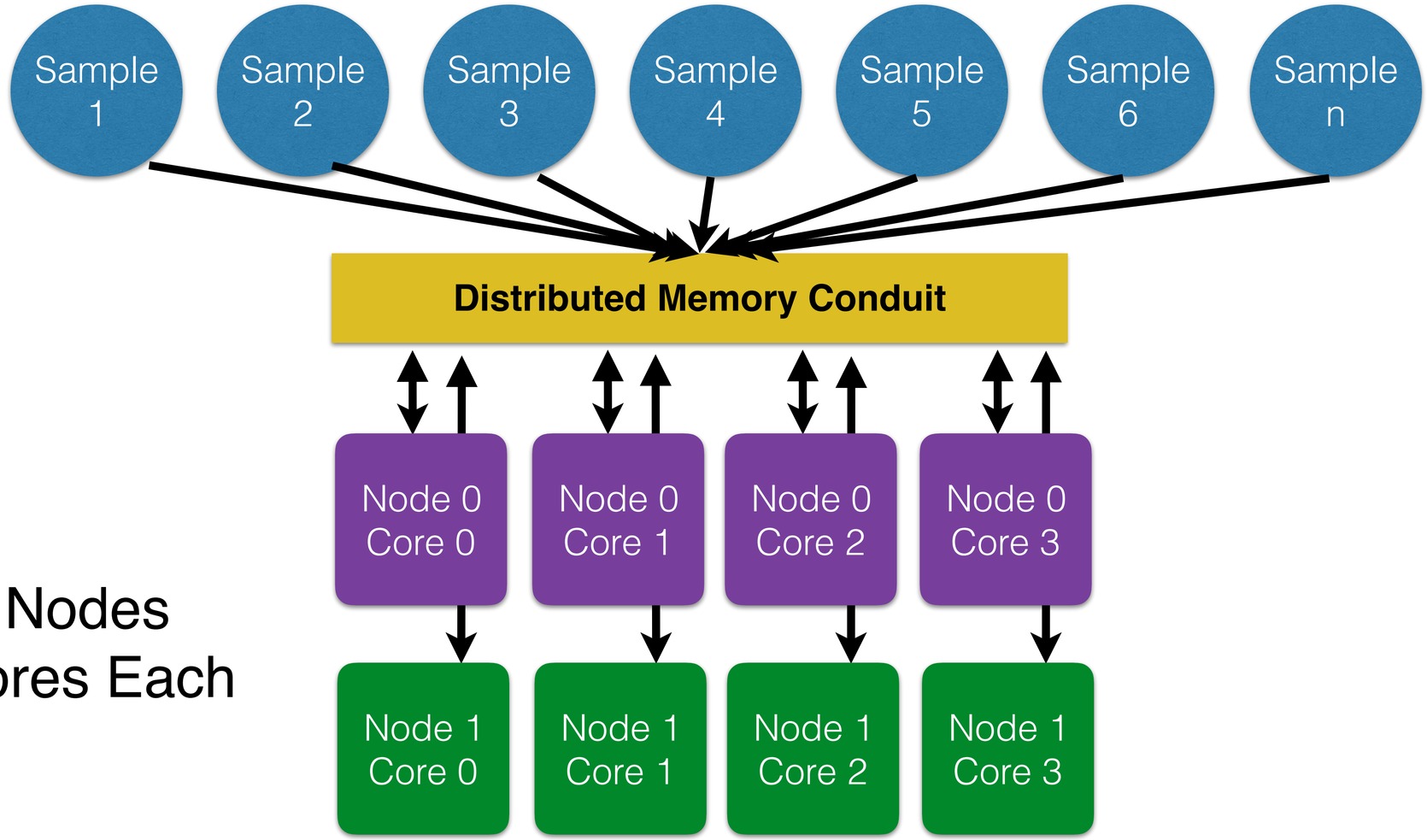
Sam

Wasted Resources

Time

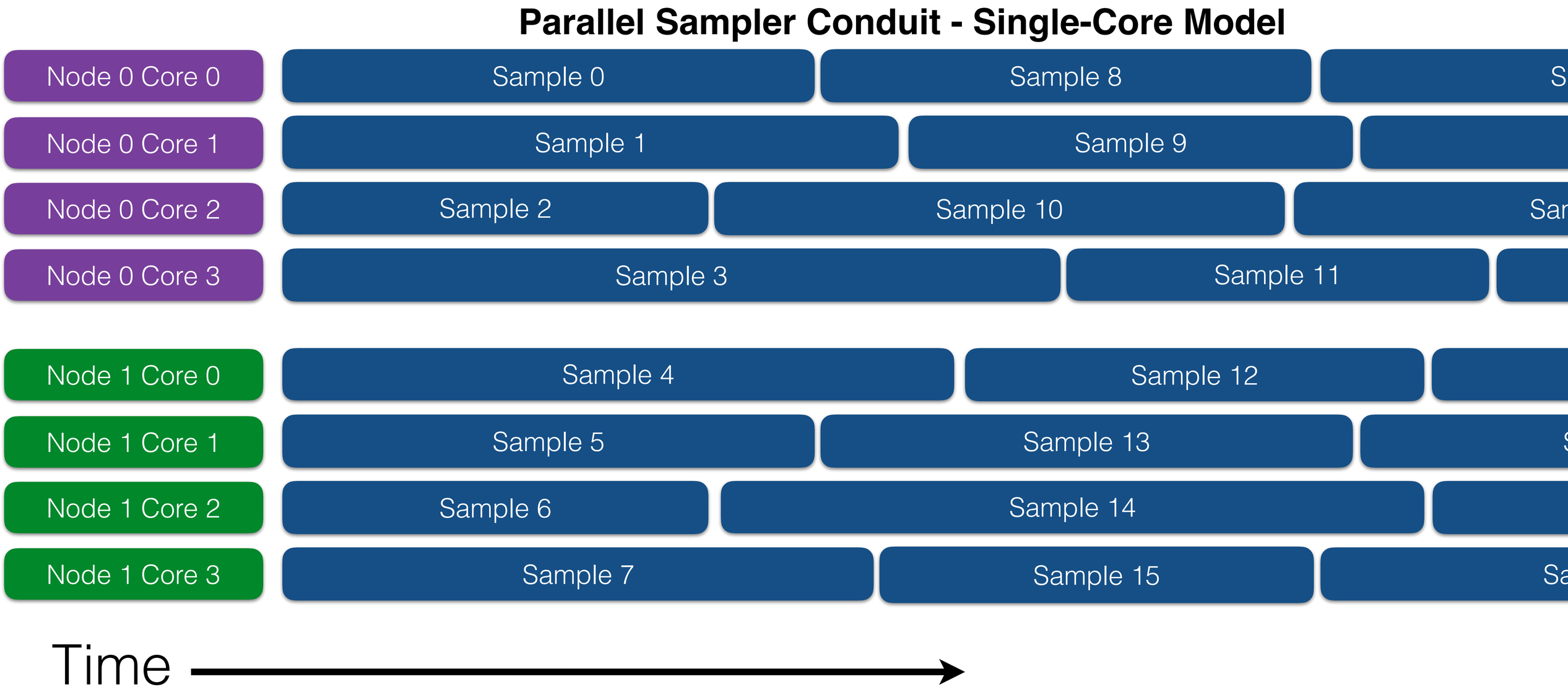
Module: Distributed Memory Conduit

Sample Population (Generation 0)



2 Nodes
4 Cores Each

High Throughput Computing

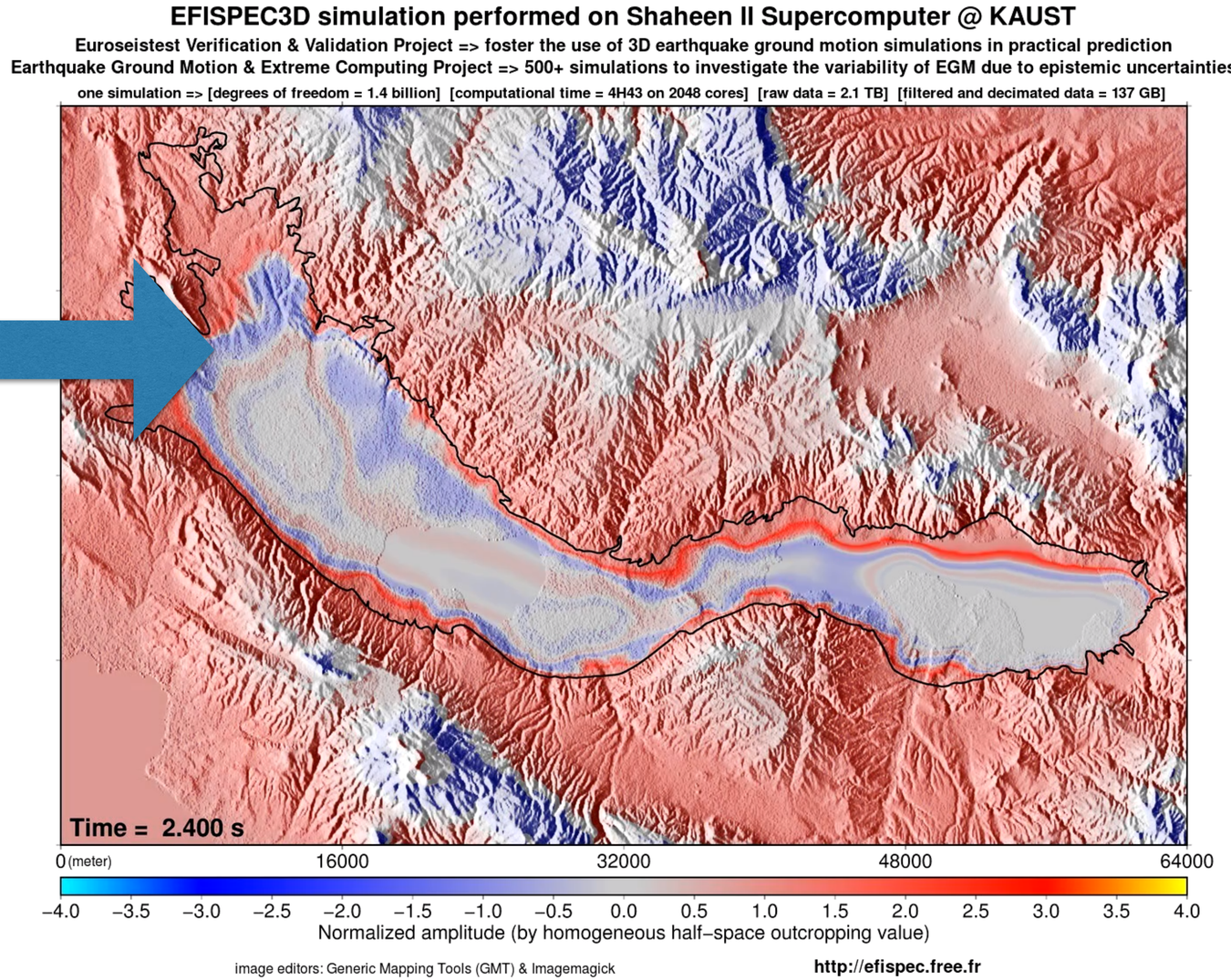


Perfectly (Embarassingly) Parallel - Independent samples & No Communication Costs

High Throughput (Example)

Study the variability and uncertainties of Earthquake Ground Motion models.

```
Vp  peak velocity of coherent pulse, cm/s    NS
Vp  peak velocity of coherent pulse, cm/s    EW
Tp  period of coherent pulse, s
Nc  cycles in coherent pulse
Tpk time to the peak of the pulse
phi phase angle of the pulse
Vr peak velocity of incoherent ground motion, cm/s  NS
Vr peak velocity of incoherent ground motion, cm/s  EW
Tau1 envelope rise time, s
Tau2 constant time, s
Tau3 envelope decay time, s
power spectrum central frequency, Hz
power spectrum bandwidth factor,
```

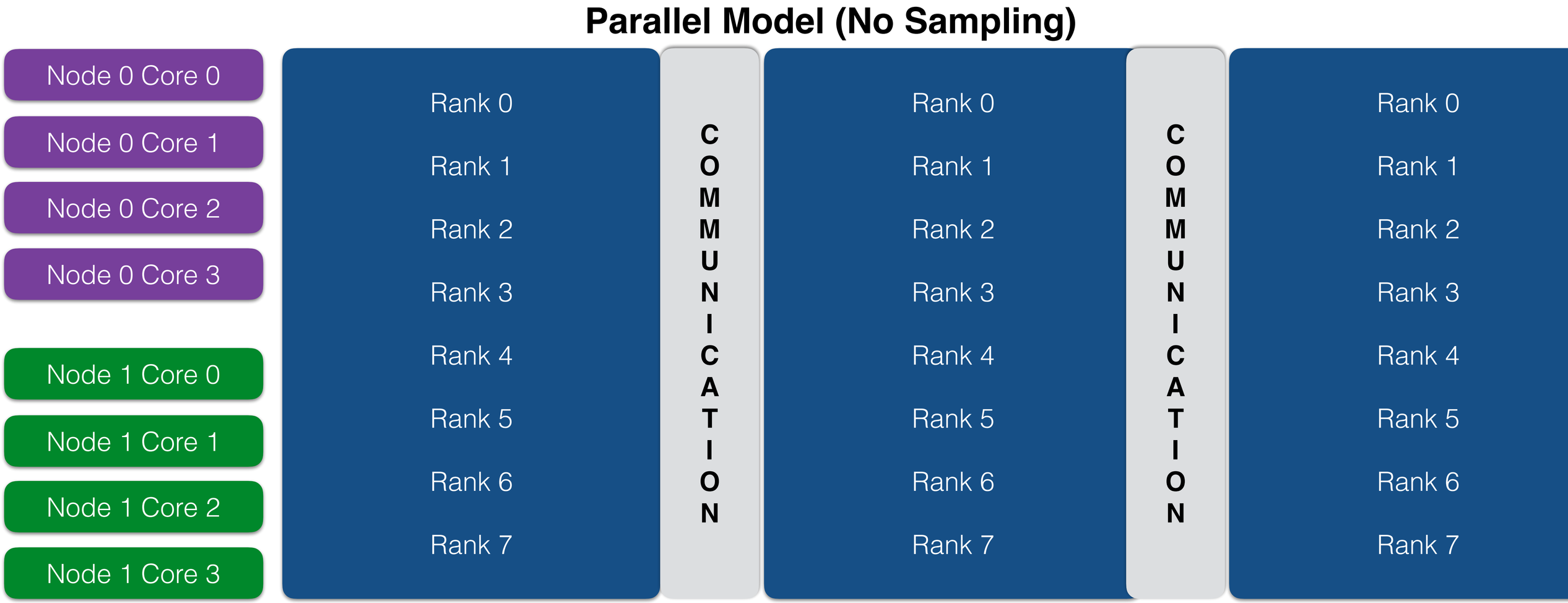


Credit: http://people.duke.edu/~hpgavin/groundmotions/

Image : https://www.brgm.eu/project/earthquake-simulations-can-uncertainties-be-quantified-more-accurently

High Performance

E.g, Iterative Solvers.

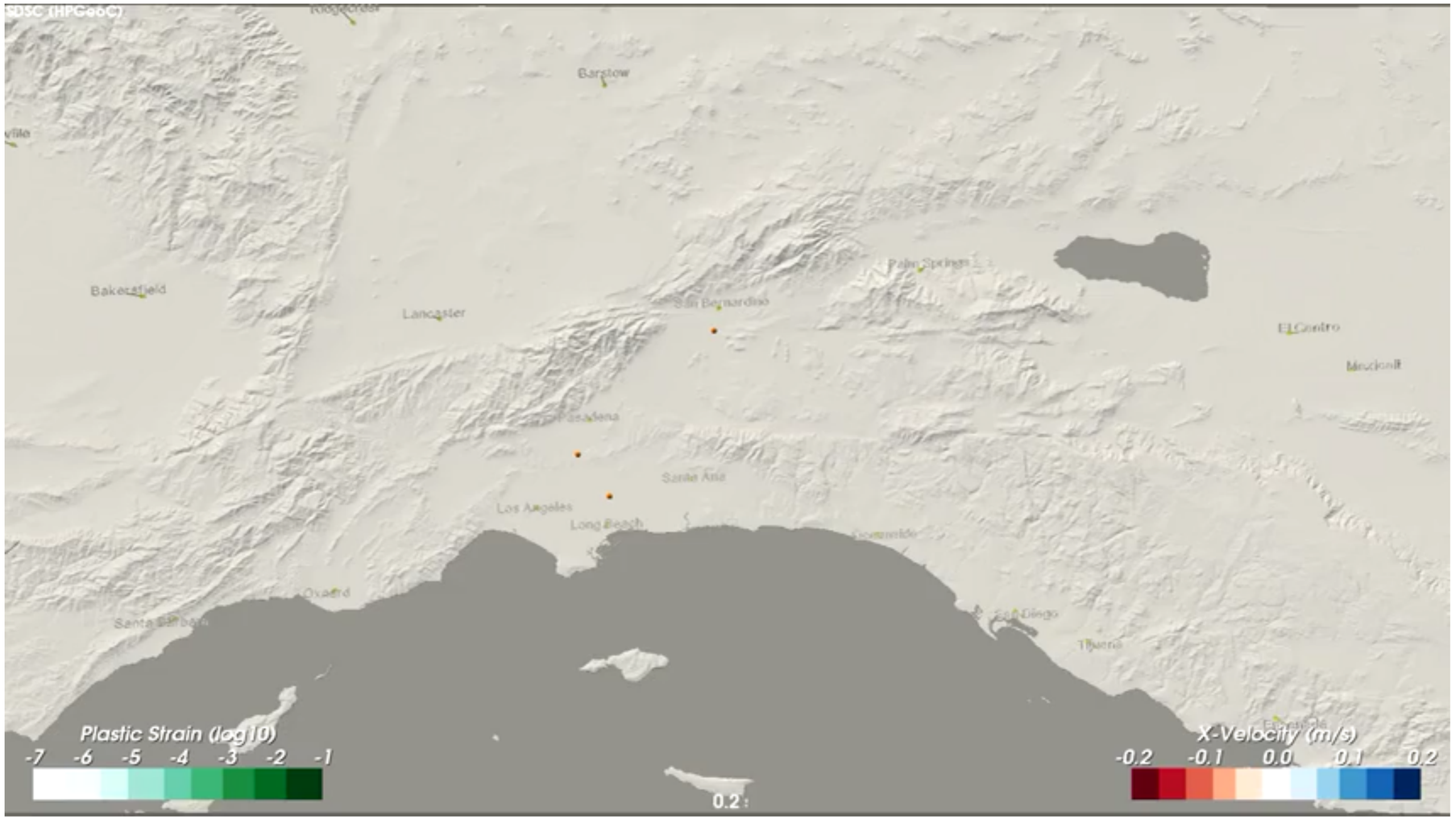


Suffers from costs of communication.

Time

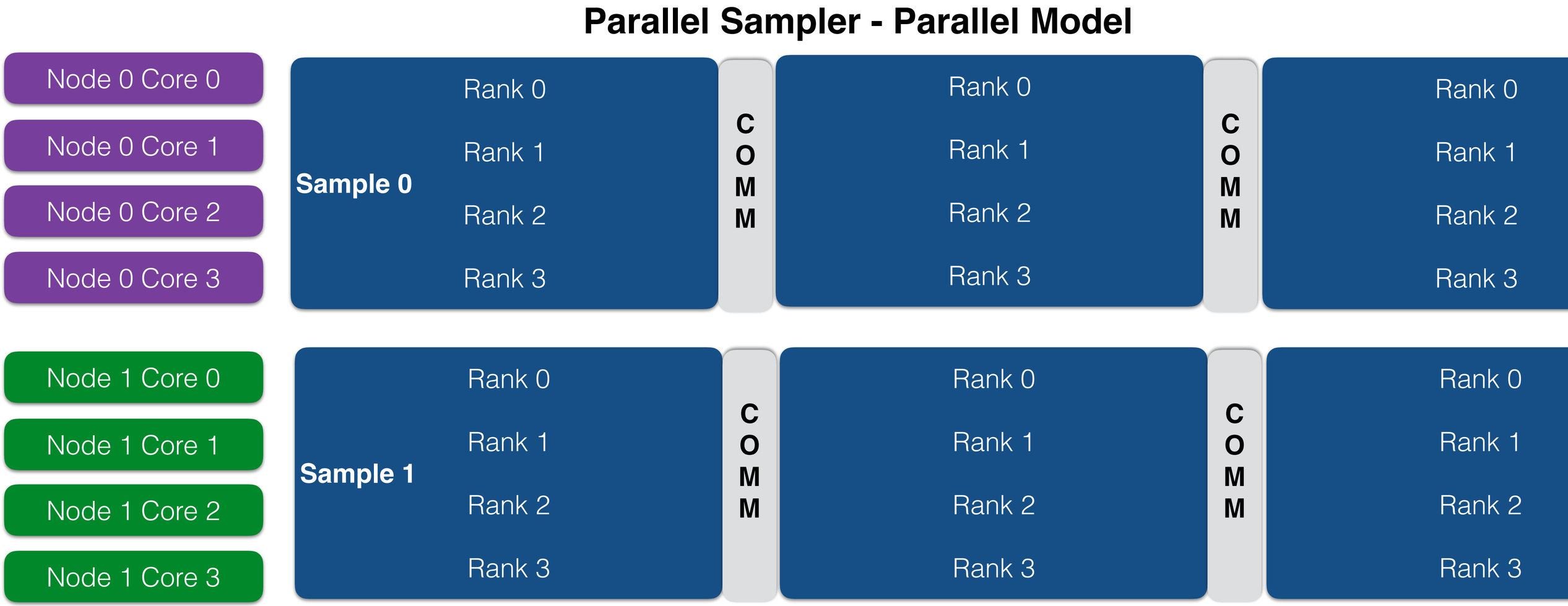
High Performance (Example)

Large-Scale simulation of Earthquake at the San Andreas fault.



Source: https://phys.org/news/2015-03-sdsc-nvidia-global-impact-award.html

Mixed Approach

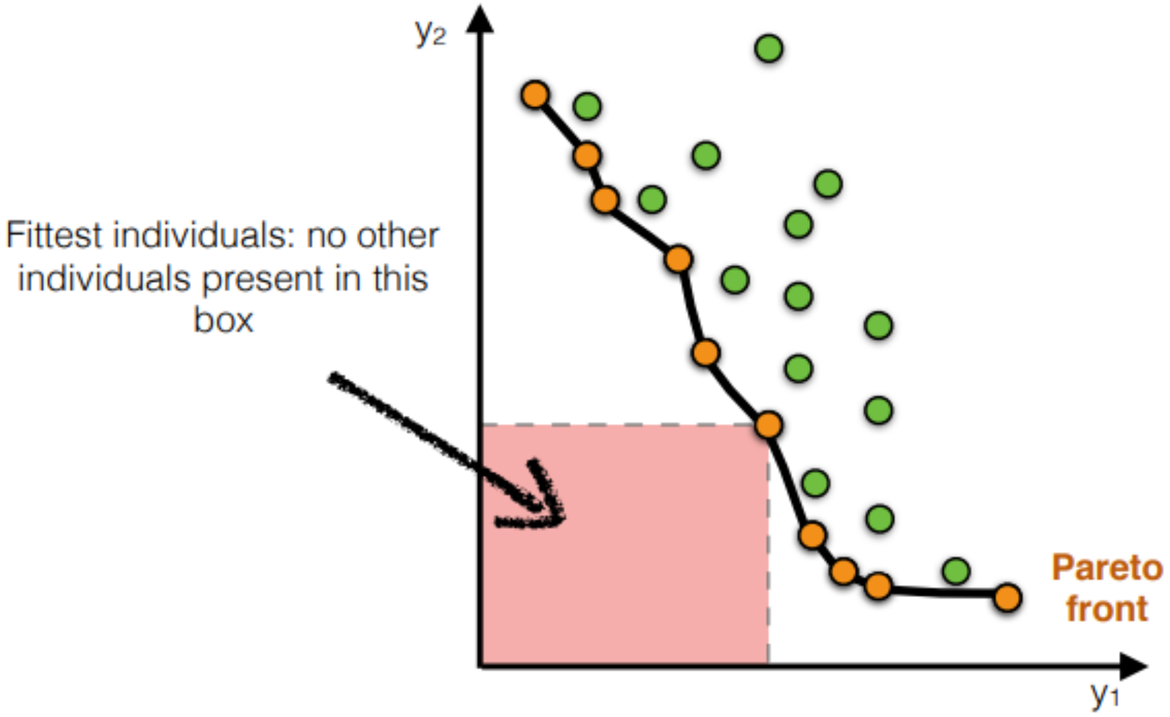


Pop Quiz: For what cases would you use parallel models & parallel sampling?

Sampling Engines
&
Tasking Strategies

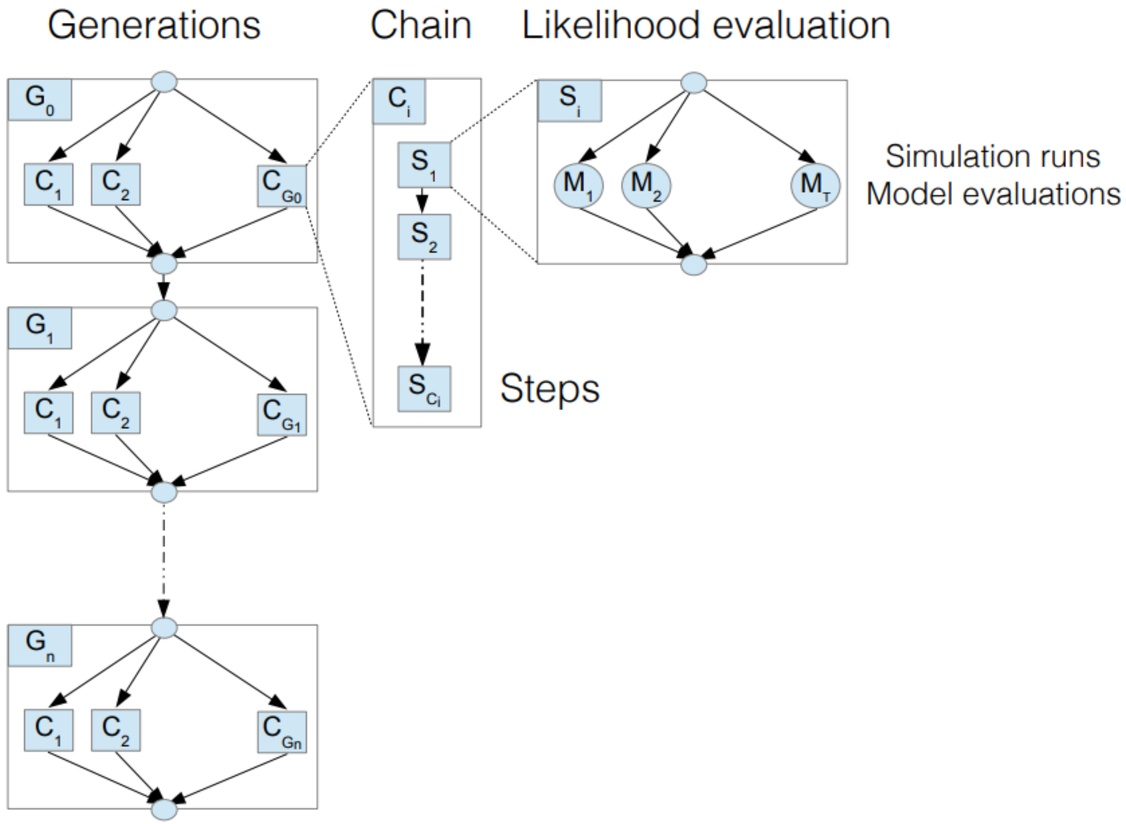
CMA-ES vs TMCMC

CMA-ES



All samples for the next generation are known at the end of the previous generation.

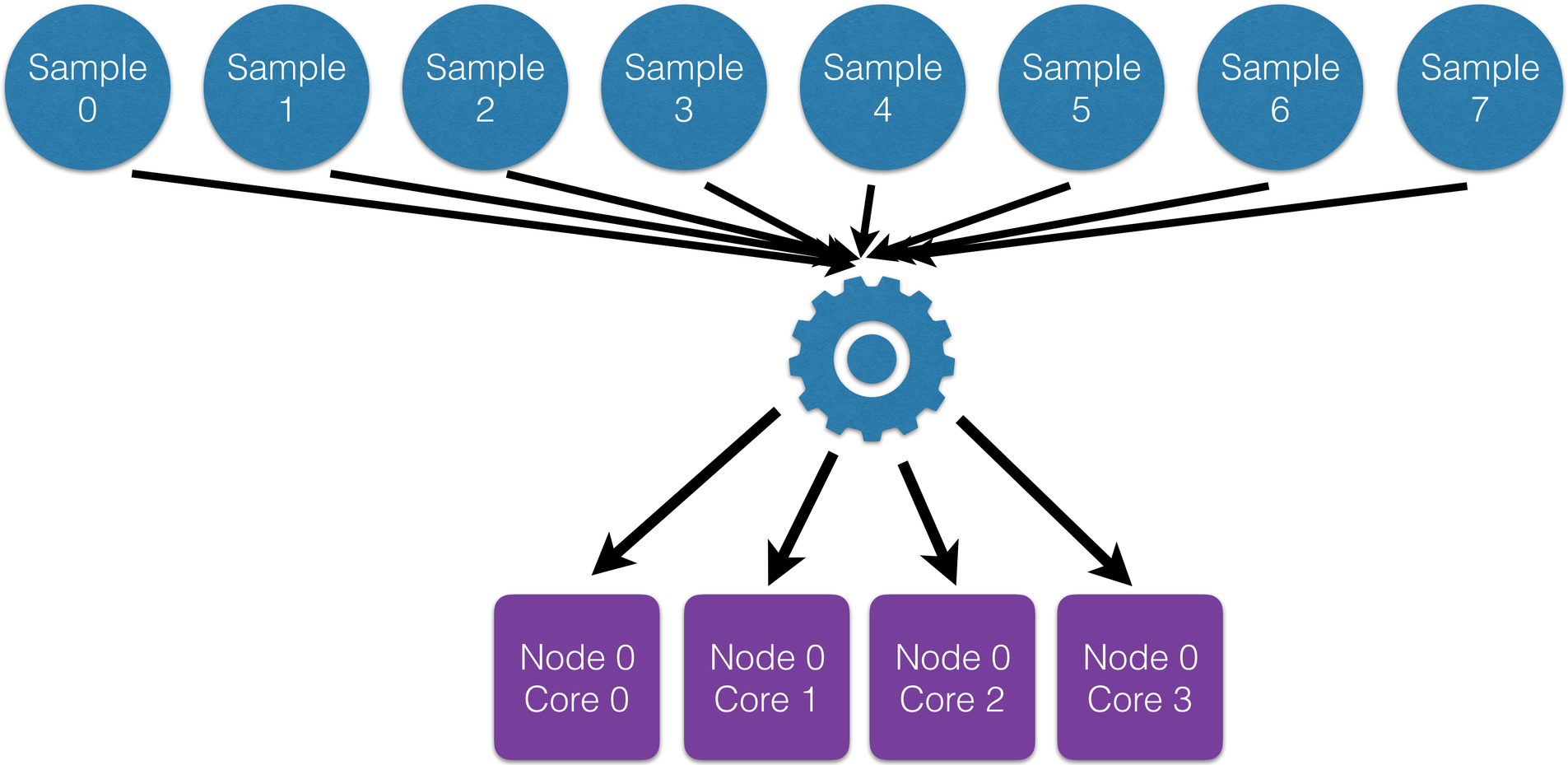
TMCMC



Samples for the current generation are determined in real-time, based on the evaluation of previous chain steps.

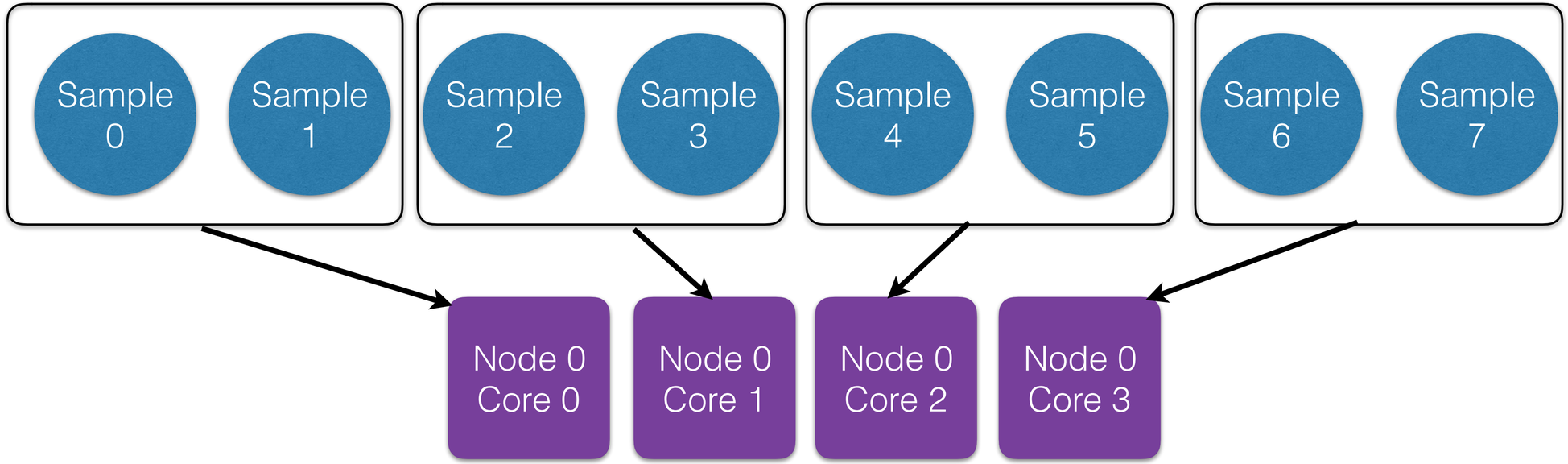
Task Distribution

How do we distribute samples to cores?



Divide-And-Conquer Strategy

Distribute samples equally (in number) among cores at the start of every generation.



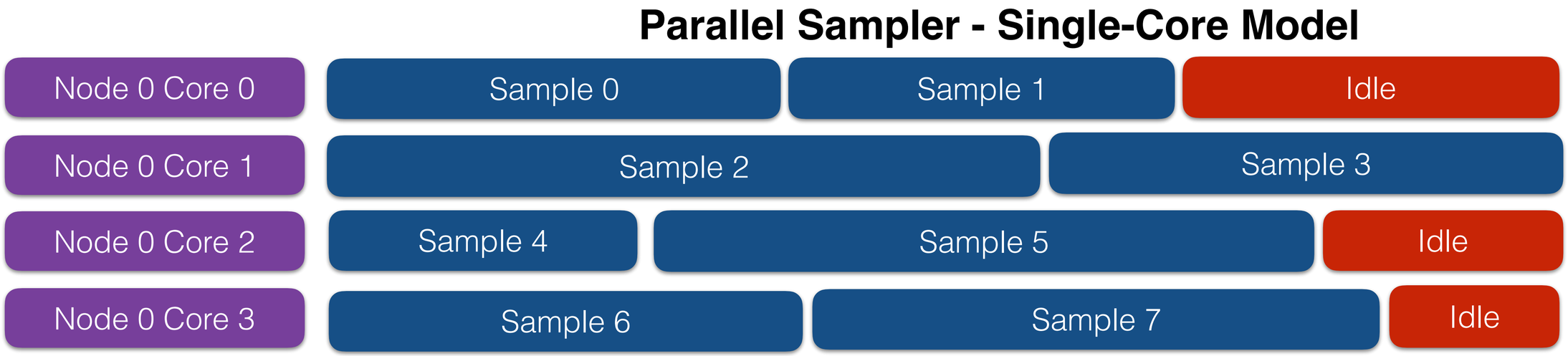
Regular communication:

- Happens at the beginning of each generation.
- Message Sizes Well-known.
- Can use separate messages or a Broadcast

Only applicable when the entire workload is known from the beginning

Load Imbalance

- Happens when cores receive uneven workloads.
- Represents a waste of computational power.

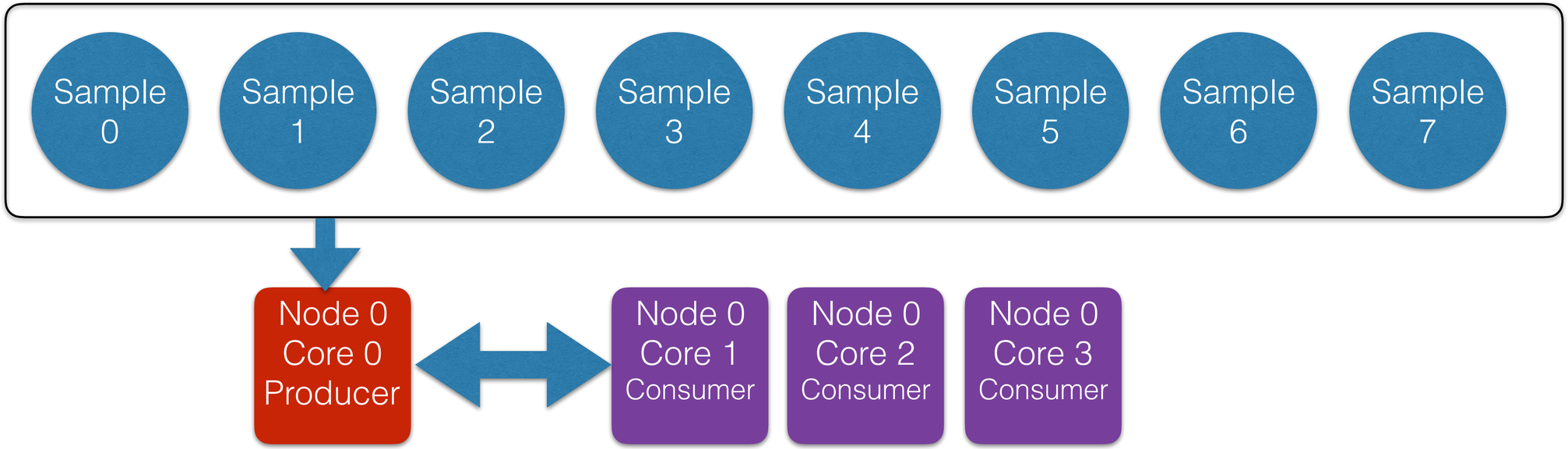


Total Running Time = Max(Core Time)

Load Imbalance Ratio = $\frac{\text{Max(Core Time)} - \text{Average(Core Time)}}{\text{Max(Core Time)}}$

Producer / Consumer Model

Assign workload opportunistically, as cores/work become available.

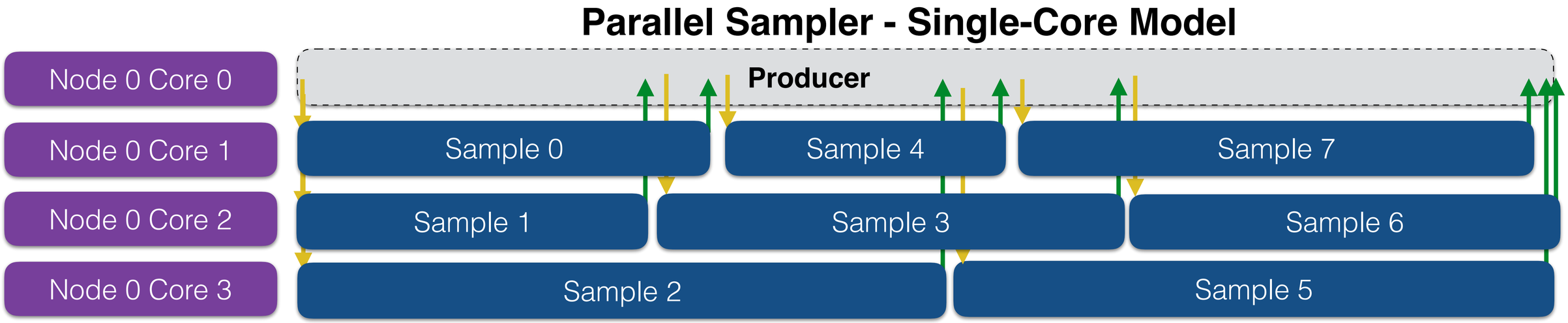


Asynchronous Behavior:

- Producer sends samples to workers as soon as they become available
- Workers *report back* finished sample and its result.
- Producer keeps a queue of available workers

Does not require the entire knowing the workload in advance.

Load Imbalance



Total Running Time ≈ Mean(Core Time), as sample size and cores → Infinite

$$\textbf{Lost Performance \%} = \frac{\#\text{ProducerCores}}{\#\text{TotalCores}}$$

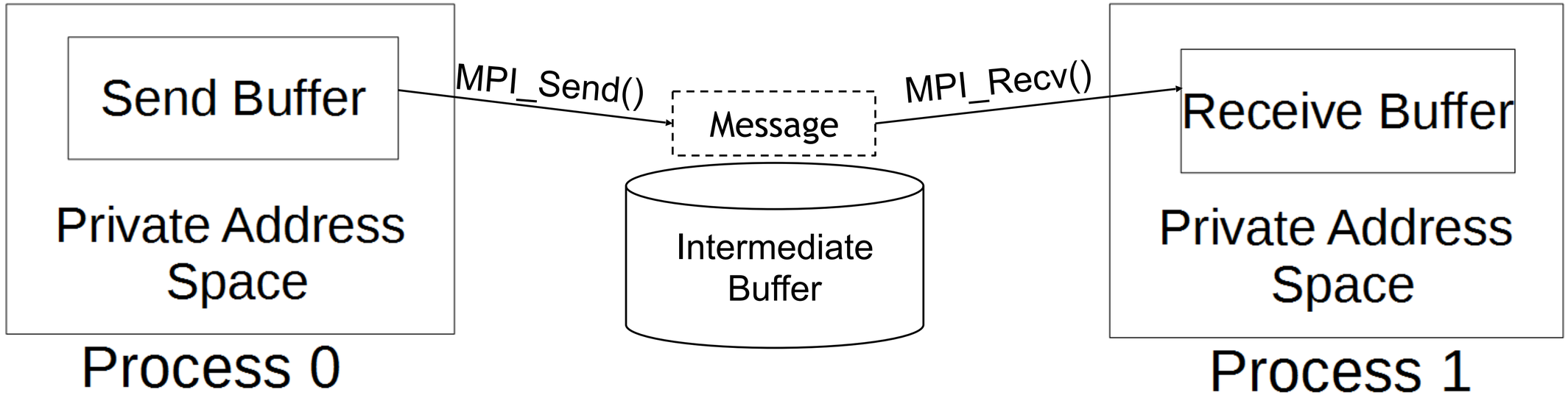
Pop Quiz: What's the impact on large multi-core systems? (Euler = 24 cores)

Message Passing Model Review

Message Passing Model

MPI: *De facto* communication standard for high-performance scientific applications.

Two-sided Communication: A sender and a receive process explicitly participate in the exchange of a message



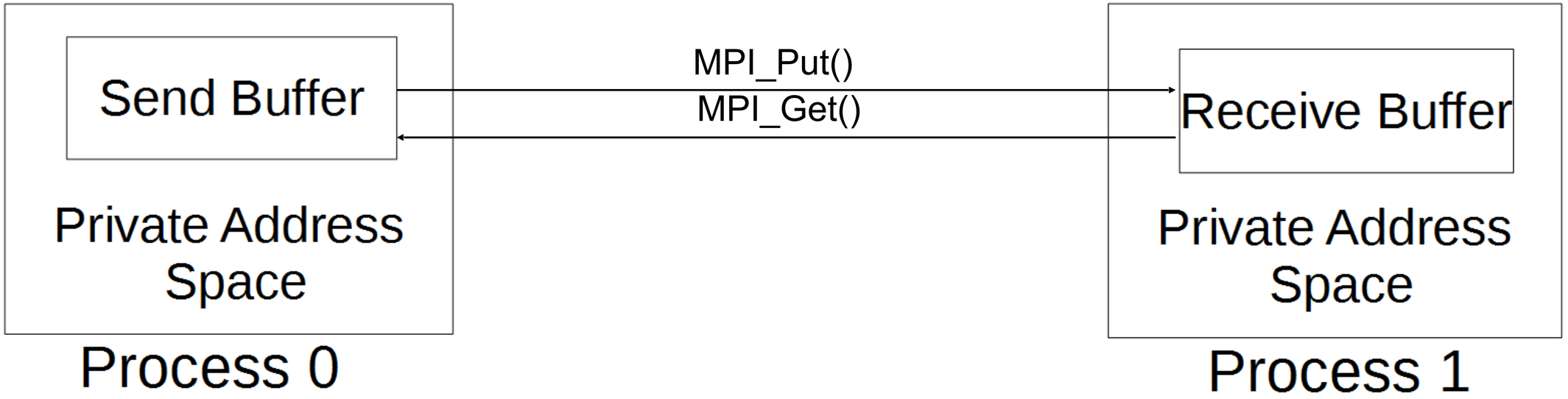
A message encodes two pieces of information:

1. The actual message payload (data)
2. The fact that two ranks reached the exchange point (synchronization).

It does not encode **semantics**: the receiver needs to know what to do with the data.

Message Passing Model

One-sided Communication: A process can directly access a shared partition in another address space



It only encodes one piece of information: **data**.

Allows passing/receiving data without a corresponding send/recv request.

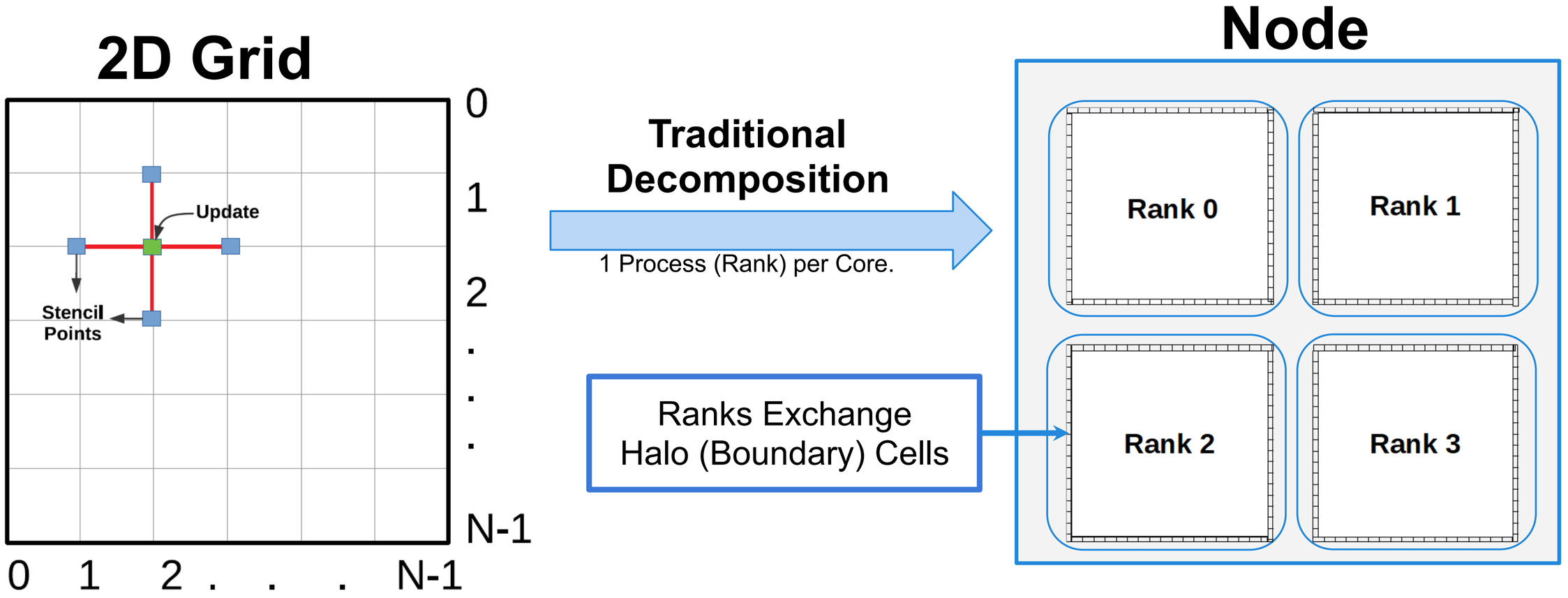
The other end is not notified of the operation (concurrency hazards)

Good for cases in which synchronization / ordering is not necessary.

A Good Case for MPI: Iterative Solvers

Structured Grid Stencil Solver

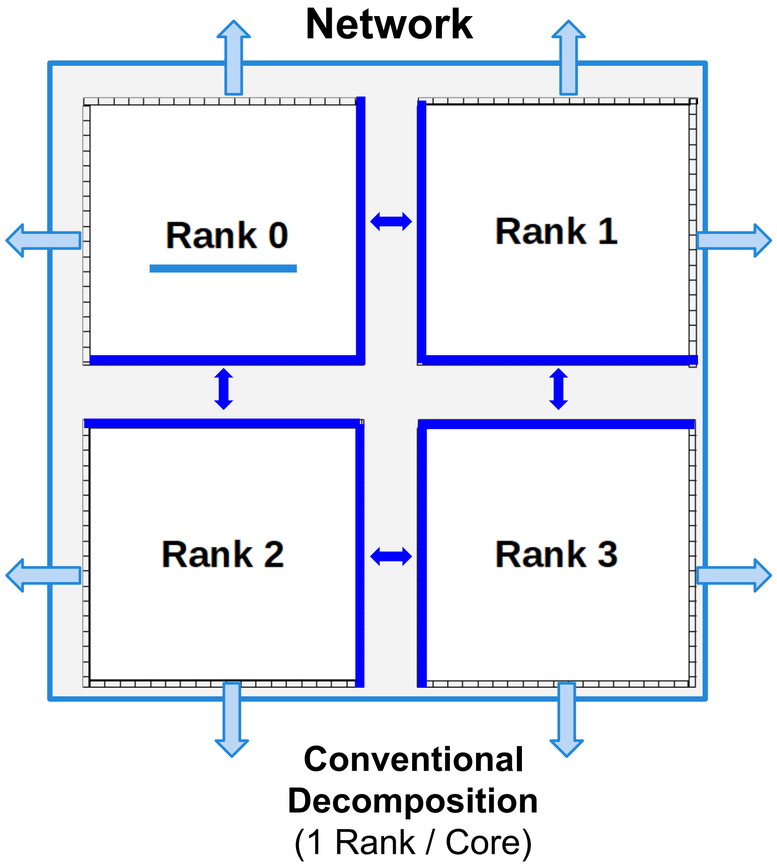
- Iteratively approaches a solution.

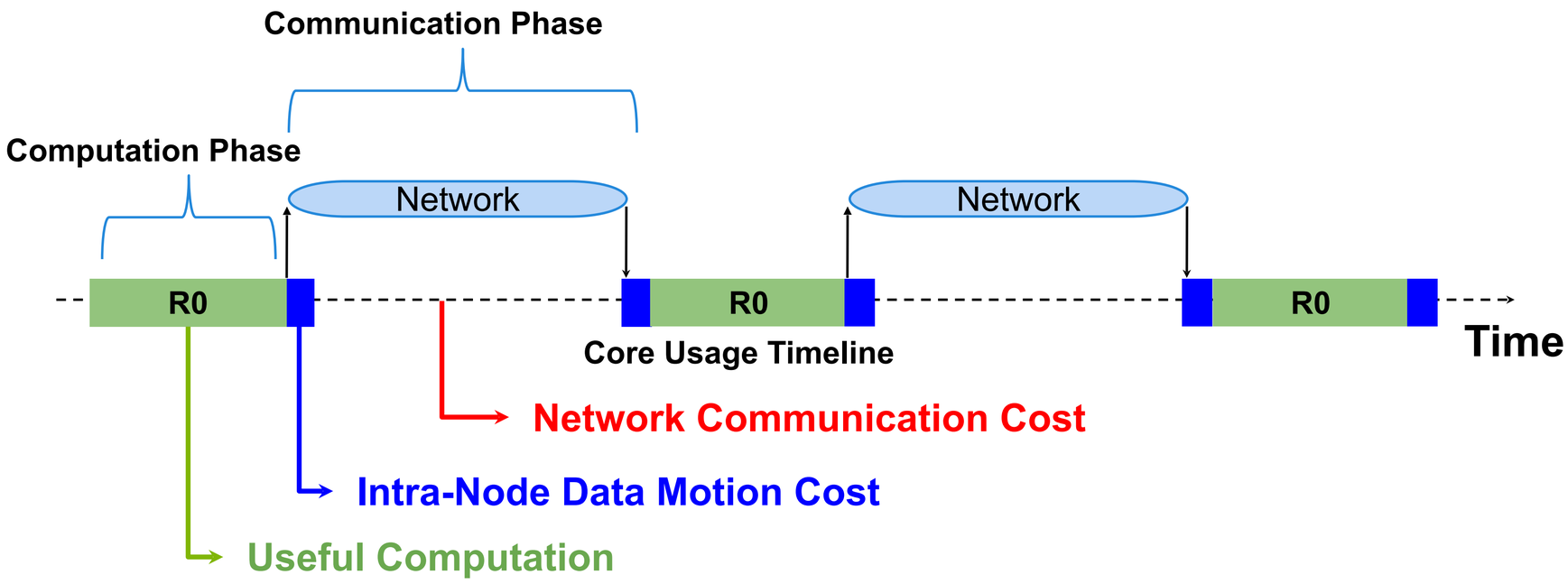


Regular Communication

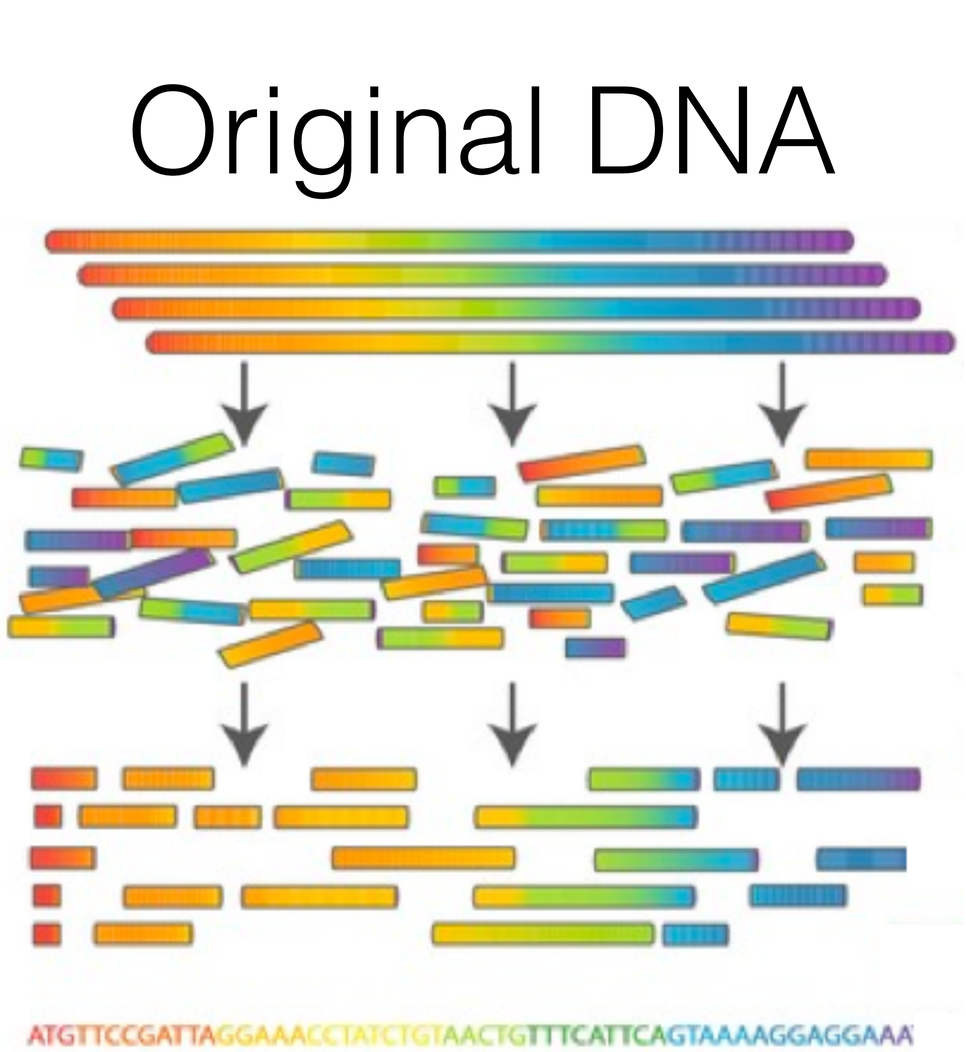
Most HPC applications are programmed under the *Bulk-Synchronous* Model.

- Iterates among separate *computation* and *communication* phases.





A NOT so Good Case for MPI: Genome Assembly



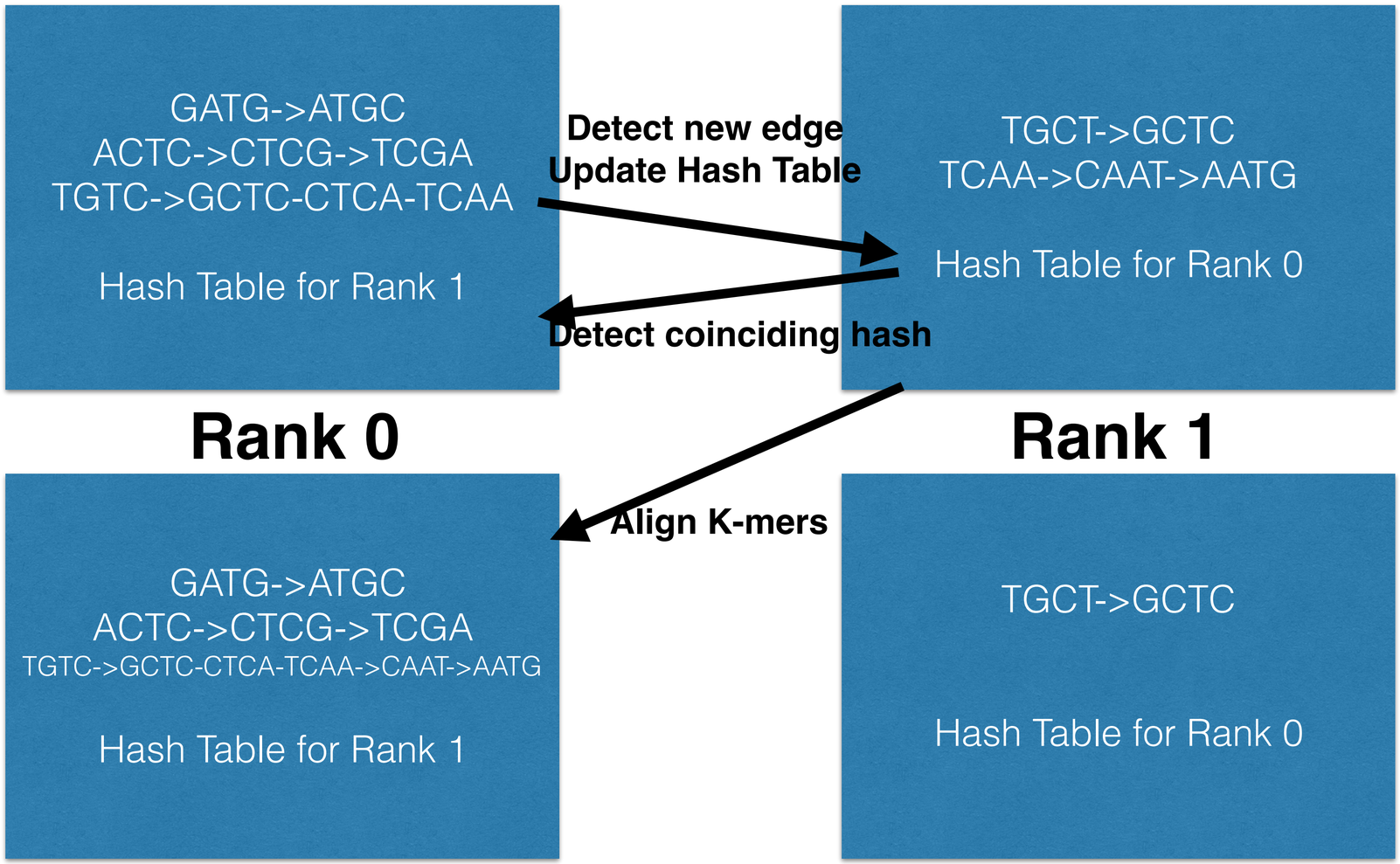
- Construct a genome (chromosome) from a pool of short fragments produced by sequencers
- Analogy: shred many copies of a book, and reconstruct the book by examining the pieces
- Complications: shreds of other books may be intermixed, can also contain errors
- Chop the reads into fixed-length fragments (k-mers)
- K-mers form a De Bruijn graph, traverse the graph to construct longer sequences
- Graph is stored in a distributed hash table

Slide Credit: Scott B. Baden (Berkeley Lab)
Image Credit: http://people.mpi-inf.mpg.de/~sven/images/assembly.png

A NOT so Good Case for MPI: Genome Assembly

Build k-mer graphs from independent segments, sharing their hash numbers.

Initial Segment of DNA: **ACTCGATGCTCAATG**



Completely Asynchronous:
- Detection of coincident hashes
- Asynchronous Hash Updates

Irregular Communication:
- K-mer chain size can vary
- Need to allocate hash entries in real time (cannot pre-allocate)

Difficult to implement on MPI due to its asynchronicity

Pop Quiz: MPI for Sampling Engines

Exam question 1:

Is MPI a good model for the divide-and-conquer strategy?

Exam Question 2:

Is MPI a good model for the producer-consumer strategy?

Asynchronous Communication: UPC++

Get started with UPC++

Read our UPC++ getting started tutorial:
https://www.cse-lab.ethz.ch/wp-content/uploads/2019/03/hpcse2-19_UPCXXTutorial.pdf

Download UPC++ Programmer's Guide, for reference:
https://bitbucket.org/berkeleylab/upcxx/wiki/Home

Run and analyze the full code of the following slides, download the codes:

- example0.cpp - Lambda Function
- example1.cpp - Hello World
- example2.cpp - Barriers
- example3.cpp - Blocking Broadcast
- example4.cpp - Non-blocking Broadcast
- example5.cpp - Single-Partition Global Memory Access
- example6.cpp - RPC with lambda functions
- example7.cpp - RPC with Quiescense (Fire-and-Forget)
- example8.cpp - Nested RPCs
- example9.cpp - Conjoining Futures
- example10.cpp - RPCs with Return Values
- example11.cpp - Global Memory with Distributed Objects

Before we start: C++ Lambda Expressions

Also known as: Anonymous Functions

What they are: Functions described as Expressions -> Convenient Notation

```
double square(double x) {  return x*x; } // Traditional Function

auto squareLambda = [](double x) -> double { return x*x; };  // Lambda Expression
```


```
int main(int argc, char* argv[])
{
  const double scale = 2.0;
  auto squareLambda = [scale](double x) -> double { return scale*x*x; };
  for (double x = 0.0; x < 5.0; x += 1.0)
     printf("X = %f, %f*X^2 = %f\n", (double)x, scale, squareLambda(x));
}
```

```
./example0
X = 0.000000, 2.000000*X^2 = 0.000000
X = 1.000000, 2.000000*X^2 = 2.000000
X = 2.000000, 2.000000*X^2 = 8.000000
X = 3.000000, 2.000000*X^2 = 18.000000
X = 4.000000, 2.000000*X^2 = 32.000000
```

>> UPC++ Intro Slides <<

UPC++ Hello World

```
#include <stdio.h>
#include <upcxx/upcxx.hpp>

int main(int argc, char* argv[])
{
  upcxx::init();
  rankId    = upcxx::rank_me();
  rankCount = upcxx::rank_n();

  printf("Hello, I am rank %d of %d\n", rankId, rankCount);

  upcxx::finalize();
  return 0;
}
```

```
>upcxx-run -n 8 ./example1
Hello, I am rank 5 of 8
Hello, I am rank 3 of 8
Hello, I am rank 7 of 8
Hello, I am rank 1 of 8
Hello, I am rank 0 of 8
Hello, I am rank 4 of 8
Hello, I am rank 6 of 8
Hello, I am rank 2 of 8
```

UPC++ Barriers

```
int main(int argc, char* argv[])
{
    upcxx::init();
    int rankId    = upcxx::rank_me();
    int rankCount = upcxx::rank_n();

    printf("Rank %d: Let's do this first.\n", rankId);

    upcxx::barrier();

    printf("Rank %d: Let's do this second.\n", rankId);

  upcxx::finalize();
    return 0;
}
```

```
Rank 2: Let's do this first.
Rank 3: Let's do this first.
Rank 5: Let's do this first.
Rank 1: Let's do this first.
Rank 0: Let's do this first.
Rank 6: Let's do this first.
Rank 7: Let's do this first.
Rank 4: Let's do this first.
Rank 0: Let's do this second.
Rank 1: Let's do this second.
Rank 4: Let's do this second.
Rank 2: Let's do this second.
Rank 6: Let's do this second.
Rank 5: Let's do this second.
Rank 3: Let's do this second.
Rank 7: Let's do this second.
```

UPC++ (Blocking) Broadcast

```
#include <stdio.h>
#include <upcxx/upcxx.hpp>

int main(int argc, char* argv[])
{
    upcxx::init();
    int rankId    = upcxx::rank_me();
    int rankCount = upcxx::rank_n();

    int number = 0;
    if (rankId == 0) number = 500;

    upcxx::broadcast(&number, 1 /*Count*/, 0 /*Root*/).wait();

    printf("Rank %d: Number is %d.\n", rankId, number);

  upcxx::finalize();
    return 0;
}
```

```
>upcxx-run -n 8 ./example3
Rank 4: Number is 500.
Rank 0: Number is 500.
Rank 1: Number is 500.
Rank 2: Number is 500.
Rank 3: Number is 500.
Rank 5: Number is 500.
Rank 6: Number is 500.
Rank 7: Number is 500.
```

UPC++ (Non-Blocking) Broadcast

```
auto future = upcxx::broadcast(&number, 1 /*Count*/, 0 /*Root*/);

printf("Rank %d: (Before) Number is %d.\n", rankId, number);

// Do other stuff

future.wait();

printf("Rank %d: (After) Number is %d.\n", rankId, number);
```

```
>upcxx-run -n 8 ./example4
Rank 2: (Before) Number is 0.
Rank 1: (Before) Number is 0.
Rank 3: (Before) Number is 0.
Rank 6: (Before) Number is 0.
Rank 5: (Before) Number is 0.
Rank 7: (Before) Number is 0.
Rank 0: (Before) Number is 500.
Rank 4: (Before) Number is 0.
Rank 0: (After) Number is 500.
Rank 1: (After) Number is 500.
Rank 4: (After) Number is 500.
Rank 5: (After) Number is 500.
Rank 6: (After) Number is 500.
Rank 7: (After) Number is 500.
Rank 2: (After) Number is 500.
Rank 3: (After) Number is 500.
```

Accessing the Global Address Space (I)

Broadcasting the global pointer to a single partition.

```
upcxx::global_ptr<int> gptr;
if (rankId == 0) gptr = upcxx::new_array<int>(rankCount);

upcxx::broadcast(&gptr, 1, 0).wait();

auto future = upcxx::rput(&rankId, gptr + rankId, 1);

printf("Rank %d - Updating the global allocation.\n", rankId);

future.wait();

upcxx::barrier();

if (rankId == 0)
{
 int* lptr = gptr.local();
 printf("{");
 for (int i = 0; i < rankCount; i++)
  printf("%d,", lptr[i]);
 printf("}\n");
}
```

```
>upcxx-run -n 8 ./example5
Rank 0 - Updating the global allocation.
Rank 1 - Updating the global allocation.
Rank 2 - Updating the global allocation.
Rank 4 - Updating the global allocation.
Rank 3 - Updating the global allocation.
Rank 5 - Updating the global allocation.
Rank 6 - Updating the global allocation.
Rank 7 - Updating the global allocation.
{0,1,2,3,4,5,6,7,}
```

Accessing the Global Address Space (II)

Accessing multiple partitions via a distributed object.

```
auto myPartition = upcxx::new_<double>(rankId);
upcxx::dist_object<upcxx::global_ptr<double>> partitions(myPartition);

*myPartition.local() = sqrt((double)rankId);

upcxx::barrier();

if (rankId == 0) for (int i = 0; i < rankCount; i++)
{
    auto partition = partitions.fetch(i).wait();
    double val = upcxx::rget(partition).wait();
    printf("SquareRoot(%f) = %f\n", (double)i, val);
}
```

```
>upcxx-run -n 8 ./example11
SquareRoot(0.000000) = 0.000000
SquareRoot(1.000000) = 1.000000
SquareRoot(2.000000) = 1.414214
SquareRoot(3.000000) = 1.732051
SquareRoot(4.000000) = 2.000000
SquareRoot(5.000000) = 2.236068
SquareRoot(6.000000) = 2.449490
SquareRoot(7.000000) = 2.645751
```

Asynchronous Execution with RPCs

Remote Procedure Call - Using Lambda Expressions.

```
upcxx::init();
rankId    = upcxx::rank_me();
int rankCount = upcxx::rank_n();

finished = false;
upcxx::barrier();

if (rankId == 0)
    for (int i = 1; i < rankCount; i++)
        upcxx::rpc(i, [](int par){
         printf("Rank %d: Received RPC with Parameter: %d\n", rankId, par);
         finished = true;
       }, i*rankCount).wait();

if (rankId > 0) while (!finished) upcxx::progress();
```

```
>upcxx-run -n 8 ./example6
Rank 1: Received RPC with Parameter: 8
Rank 2: Received RPC with Parameter: 16
Rank 3: Received RPC with Parameter: 24
Rank 4: Received RPC with Parameter: 32
Rank 5: Received RPC with Parameter: 40
Rank 6: Received RPC with Parameter: 48
Rank 7: Received RPC with Parameter: 56
```

Conjoining Futures

So that we can continue doing stuff while they finish

```
upcxx::future<> futs = upcxx::make_future();

if (rankId == 0)
  for (int i = 1; i < rankCount; i++)
  {
   auto fut = upcxx::rpc(i, [](int par){
     printf("Rank %d: Received RPC with Parameter: %d\n", rankId, par);
     finished = true;
    }, i*rankCount);
   futs = upcxx::when_all(futs, fut);
  }

if (rankId > 0) while (!finished) upcxx::progress();

if (rankId == 0) printf("Not all finished yet.\n");
  if (rankId == 0) futs.wait();
  if (rankId == 0) printf("All finished now.\n");
```

```
>upcxx-run -n 8 ./example9
Rank 1: Received RPC with Parameter: 8
Rank 2: Received RPC with Parameter: 16
Rank 3: Received RPC with Parameter: 24
Rank 4: Received RPC with Parameter: 32
Not all finished yet.
Rank 5: Received RPC with Parameter: 40
Rank 6: Received RPC with Parameter: 48
Rank 7: Received RPC with Parameter: 56
All finished now.
```

Composing Futures

Useful for defining callbacks to previous RPCs

```
if (rankId == 0)
{
 upcxx::future<> futs = upcxx::make_future();
 for (int i = 1; i < rankCount; i++)
 {
  auto f1 = upcxx::rpc(i, [](int par){
   printf("Rank %d: Received RPC with Parameter: %d\n", rankId, par);
   finished = true;
  }, i*rankCount);
  f1.then([i](){printf("Rank 0: Rank %d Came back.\n", i);});
  futs = upcxx::when_all(futs,f1);
 }
 futs.wait();
}
```

```
[upcxx-run -n 8 ./example12
Rank 1: Received RPC with Parameter: 8
Rank 3: Received RPC with Parameter: 24
Rank 6: Received RPC with Parameter: 48
Rank 4: Received RPC with Parameter: 32
Rank 7: Received RPC with Parameter: 56
Rank 5: Received RPC with Parameter: 40
Rank 2: Received RPC with Parameter: 16
Rank 0: Rank 1 Came back.
Rank 0: Rank 3 Came back.
Rank 0: Rank 6 Came back.
Rank 0: Rank 4 Came back.
Rank 0: Rank 7 Came back.
Rank 0: Rank 5 Came back.
Rank 0: Rank 2 Came back.
```

RPC with Return Values

```
int calculateSquare(int x) { return x*x; }

int main(int argc, char* argv[])
{
  upcxx::init();
  int rankId    = upcxx::rank_me();
  int rankCount = upcxx::rank_n();

  if (rankId == 0)
   for (int i = 1; i < rankCount; i++)
    printf("Value: %d - Square %d\n", i, upcxx::rpc(i, calculateSquare, i).wait());
```

```
>upcxx-run -n 8 ./example10
Value: 1 - Square 1
Value: 2 - Square 4
Value: 3 - Square 9
Value: 4 - Square 16
Value: 5 - Square 25
Value: 6 - Square 36
Value: 7 - Square 49
```

Quiescense (Fire and Forget)

When we don't need a response

```
int main(int argc, char* argv[])
{
    upcxx::init();
    rankId    = upcxx::rank_me();
    int rankCount = upcxx::rank_n();

    finished = false;
    upcxx::barrier();

    if (rankId == 0)
        for (int i = 1; i < rankCount; i++)
            upcxx::rpc_ff(i, [](int par){
             printf("Rank %d: Received RPC with Parameter: %d\n", rankId, par);
             finished = true;
          }, i*rankCount);

    if (rankId > 0) while (!finished) upcxx::progress();
```

```
>upcxx-run -n 8 ./example7
Rank 2: Received RPC with Parameter: 16
Rank 1: Received RPC with Parameter: 8
Rank 3: Received RPC with Parameter: 24
Rank 4: Received RPC with Parameter: 32
Rank 5: Received RPC with Parameter: 40
Rank 6: Received RPC with Parameter: 48
Rank 7: Received RPC with Parameter: 56
```

Nested RPCs

When the reciever also needs the sender to do something

```
upcxx::barrier();


if (rankId == 0)
 for (int i = 1; i < rankCount; i++)
  upcxx::rpc_ff(i, [](int par){
   printf("Rank %d: Received RPC with Parameter: %d\n", rankId, par);
   finished = true;
   upcxx::rpc_ff(0, []()
   {
    responses++;
    printf("Rank 0: Received responses: %d\n", responses);
    if (responses == rankCount-1) finished = true;
   });
  }, i*rankCount);
```

```
>upcxx-run -n 8 ./example8
Rank 2: Received RPC with Parameter: 16
Rank 1: Received RPC with Parameter: 8
Rank 3: Received RPC with Parameter: 24
Rank 5: Received RPC with Parameter: 40
Rank 4: Received RPC with Parameter: 32
Rank 6: Received RPC with Parameter: 48
Rank 7: Received RPC with Parameter: 56
Rank 0: Received responses: 1
Rank 0: Received responses: 2
Rank 0: Received responses: 3
Rank 0: Received responses: 4
Rank 0: Received responses: 5
Rank 0: Received responses: 6
Rank 0: Received responses: 7
```