High-Performance Computing for the simulation of particles with the Discrete Element Method

14th International SuperComputing Camp
https://sc-camp.org

SC-Camp 2023

Cartagena, Colombia
May 14-20, 2023

camp

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Outline

Introduction to High-Performance Computing

- Motivations
- Parallelization Approaches
- Memory Models and Programming Models
- Parallel Programming Caveats
- Performance Modeling and Analysis

HPC for the Simulation of Particles

- Discrete Element Method and XDEM
- Domain Decomposition and Load-Balancing
- Fine Grain Parallelization with OpenMP
- Faster Broad-Phase with Roofline Analysis
- Verlet Buffer approach for Collision Detection

Going further: DEM+CFD

- Parallel Multi-Physics Simulation of a Biomass Furnace

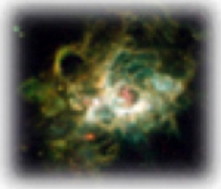
Introduction to

High-Performance Computing

Motivations

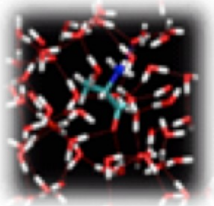
Computer Simulation is everywhere

Electro-
Magnetics

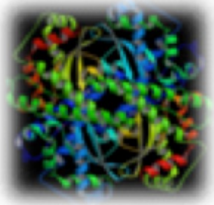


Computational Chemistry
Quantum Mechanics

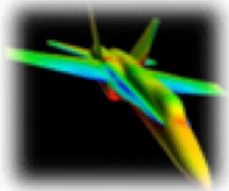
Computational Chemistry
Molecular Dynamics



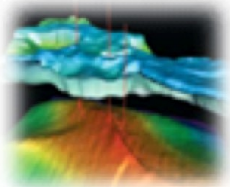
Computational
Biology



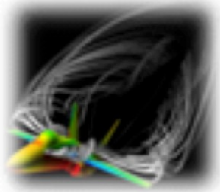
Structural Mechanics
Implicit



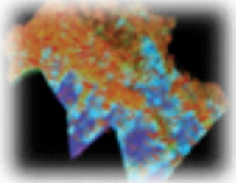
Seismic
Processing



Computational Fluid
Dynamics



Reservoir
Simulation



Rendering
Ray Tracing

Climate / Weather
Ocean Simulation

Data Analytics

Structural Mechanics
Explicit

- Computational Fluid Dynamics (OpenFOAM)
- Finite Element Analysis (Abaqus)
- Climate / Weather / Ocean Simulation (WRF)
- Molecular Dynamics (Gromacs, Amber)
- Quantum Chemistry (Quantum Espresso)
- Visualization (Paraview)
- Data processing (R, Matlab)
- ...

What is High Performance Computing?

High Performance Computing (HPC)

- Use of parallel and distributed computers with fast interconnects
- To execute an application quickly and efficiently

Why parallel computers?

- Performance of single CPU core is getting limited (power, physics)
- Multiple cores are used to increase the computing capacity

HPC is challenging

- Active research domain
- Provides tools for many other researchers

How to get faster with HPC?

~~Build faster processor~~

- Moore’s law continues but ***The free lunch is over!***
- CPU serial-processing speed is reaching its physical limit

➔ **Multi-cores processor architectures**

➔ **Accelerators and specialized processors** (GPU, TPU, FPGA, etc.)

Combine multiple computers

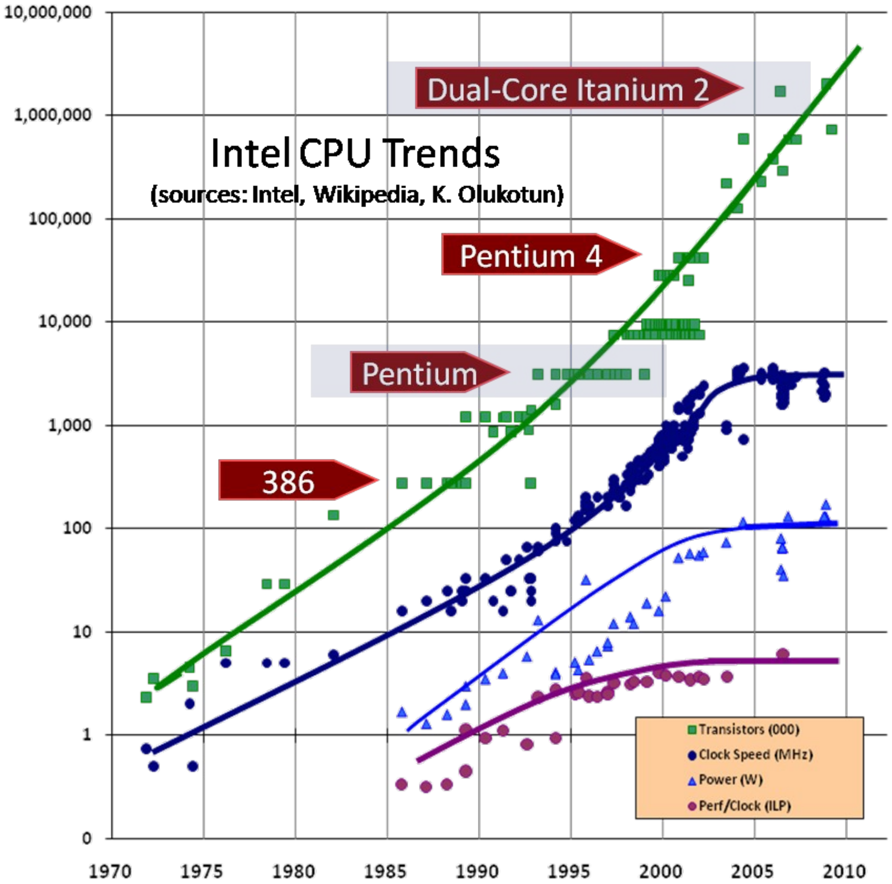
➔ **HPC Clusters and Supercomputers**

Better use of the hardware

➔ **Identify the actual bottleneck** (CPU, memory, network, etc.)

➔ **Vectorization (SIMD)**

Not to forget: **Better algorithms**



H. Sutter. *The Free Lunch Is Over*. 2005

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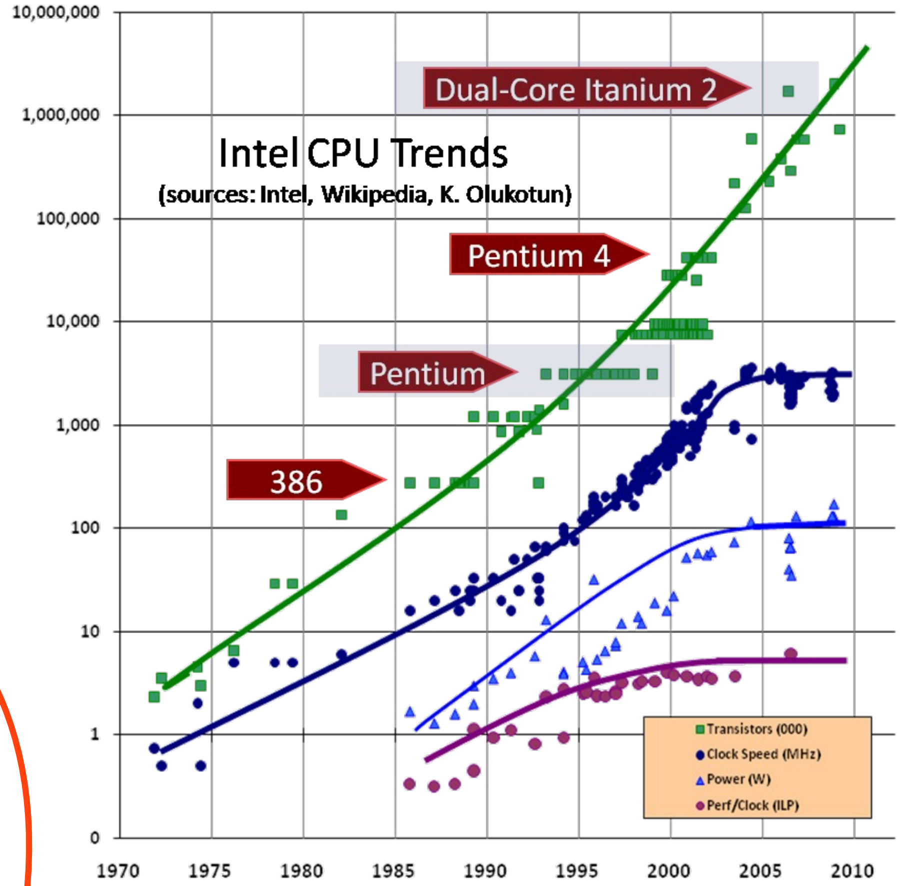


H. Sutter. *The Free Lunch Is Over*. 2005

Parallel programming

How much faster is HPC?

Your simulation is limited by the performance of you computer

	Your laptop	Uni.lu HPC*	Frontier*
CPU	4 cores	46,528 cores	602,112 cores
Memory	16 **G**B	130 **T**B	9.2 **P**B
Storage	1 **T**B	3.48 **P**B	700 **P**B
Network	Ethernet 10 Gb/s	Infiniband 100 Gb/s	Slingshot 100 GB/s
Accelerators	1 GPU	96 GPUs	37,632 GPUs
R_{peak}	350 **G**flops	1,847 **T**flops	1,686 **P**flops

* shared with other users

→ HPC provides the **methodology** and **tools** for your application to run faster

Introduction to

High-Performance Computing

Parallelization Approaches

How to parallelize an algorithm?

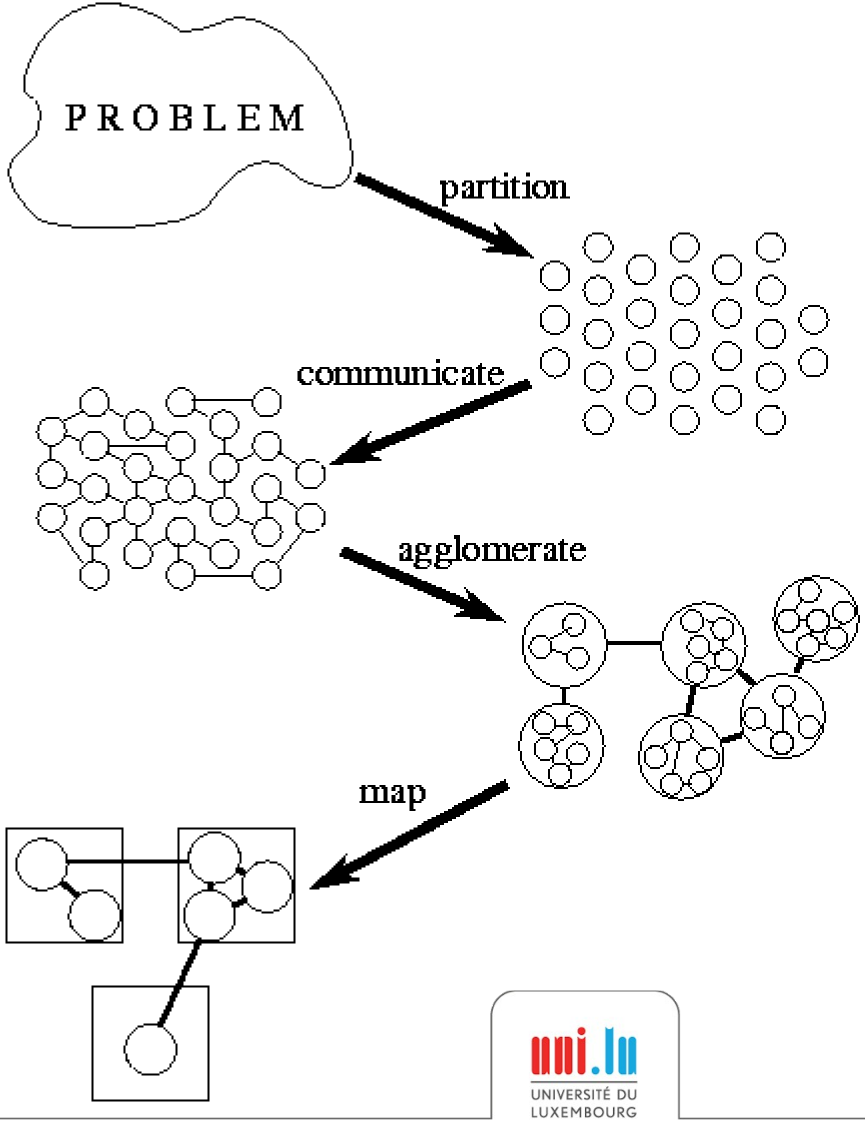
Designing and Building Parallel Programs,
by Ian Foster, 1995.

Partitioning: decompose computation in small tasks, independently of the number of processors

Communication: identify coordination and dependencies between tasks

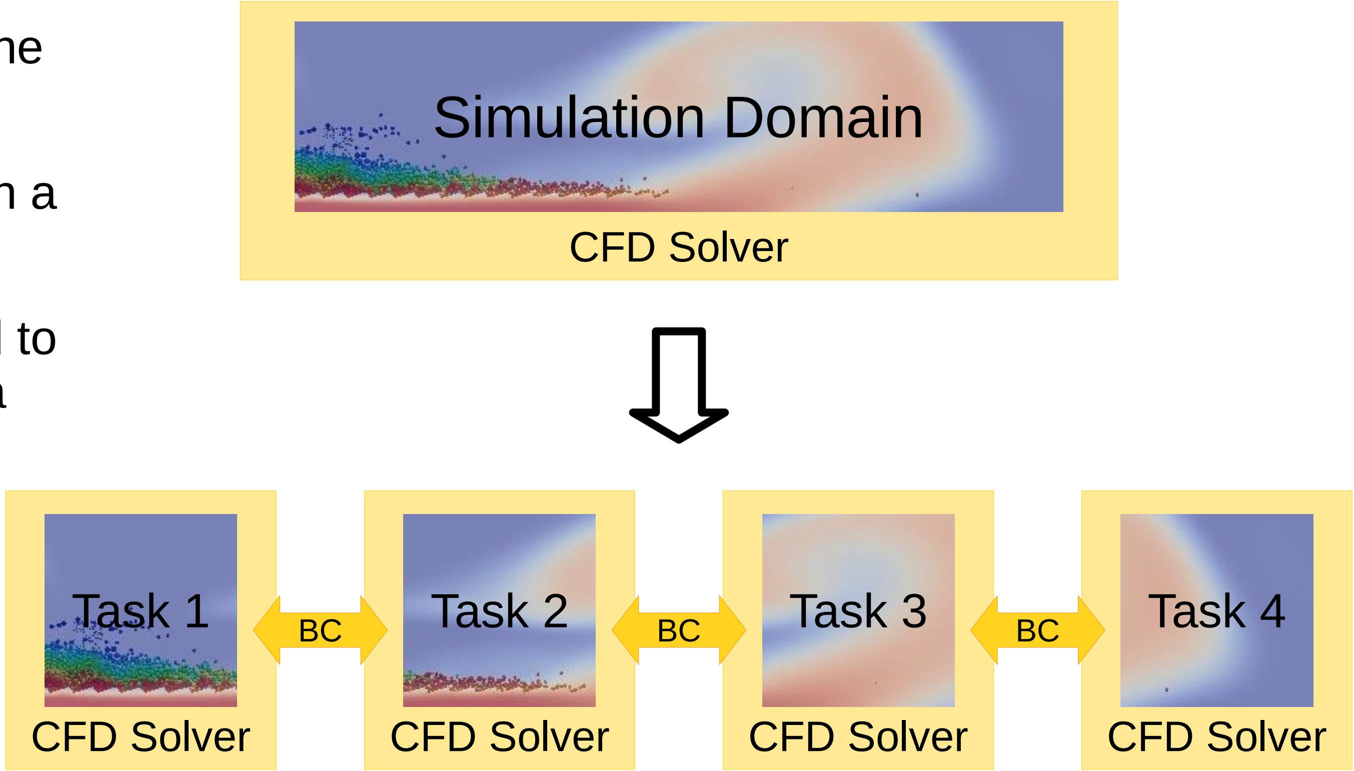
Agglomeration: tasks are combined into larger tasks to improve performance or to reduce development costs

Mapping: Assign tasks to processors in order to maximize processor utilization and minimize communication costs
→ load-balancing algorithms



Problem Partitioning → **Domain Decomposition**

- The data associated with the problem is decomposed
- Each parallel task works on a portion of the data
- The same program is used to process each piece of data
- Communication may be needed between tasks



Simulation Domain

CFD Solver

Task 1

CFD Solver

BC

Task 2

CFD Solver

BC

Task 3

CFD Solver

BC

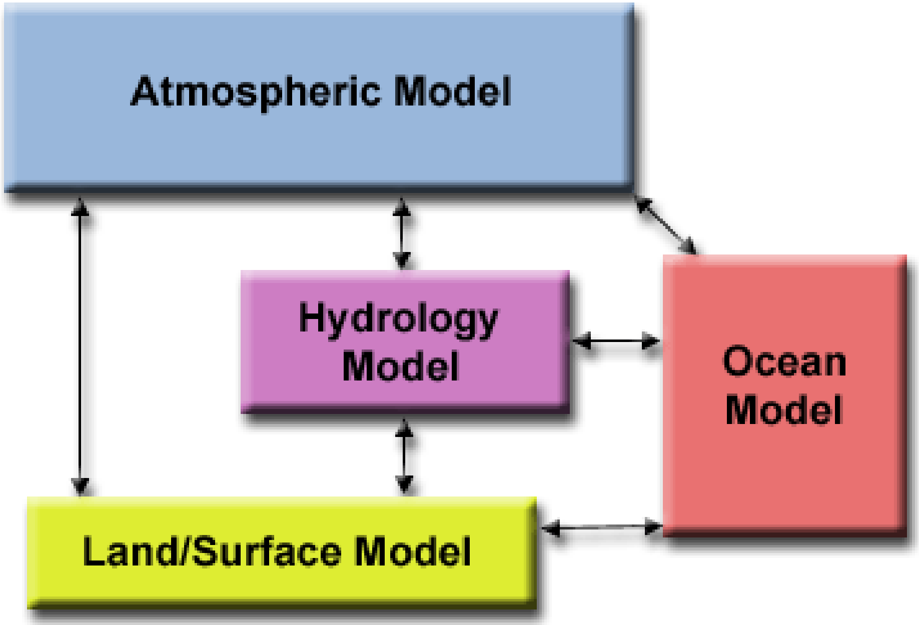
Task 4

CFD Solver

→ This is called **SPMD** for **Single Program, Multiple Data**

Problem Partitioning → **Functional Decomposition**

- Focus on the performed computation rather than on the data
- Problem decomposed according to the work to be done
- Each task then performs a portion of the overall work
- Communication may be needed between tasks



→ This is called **MPMD** for **Multiple Program, Multiple Data**

Problem Partitioning → **Functional Decomposition**

- Focus on the performed computation rather than on the data
- Problem decomposed according to the work to be done
- Each task then performs a portion of the overall work
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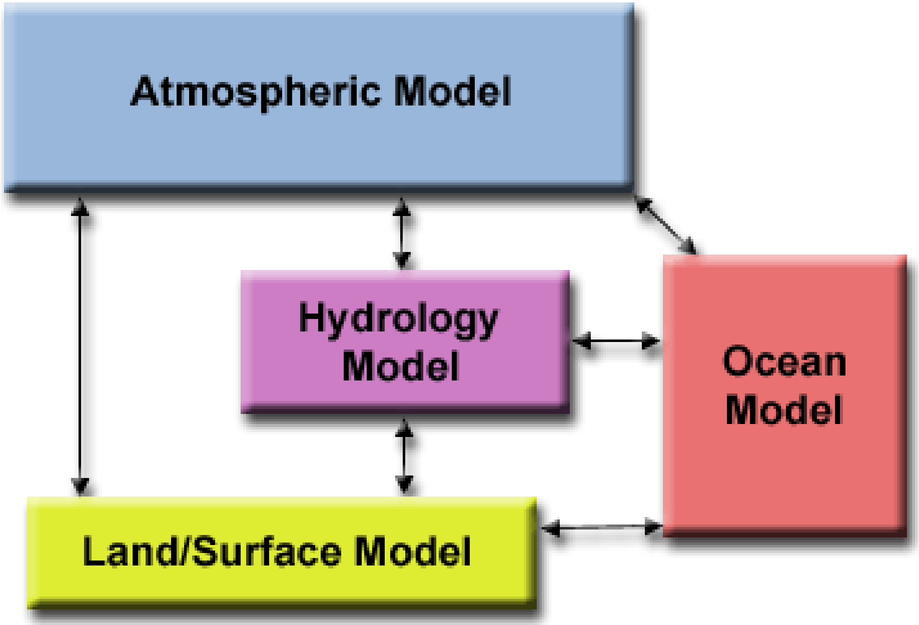


→ This is called **MPMD** for **Multiple Program, Multiple Data**

Complex applications might use an hybrid approach between Domain Decomposition and Functional Decomposition!

Introduction to

High-Performance Computing

Memory Models and Programming Models

Thread vs Process

At the level of the Operating System

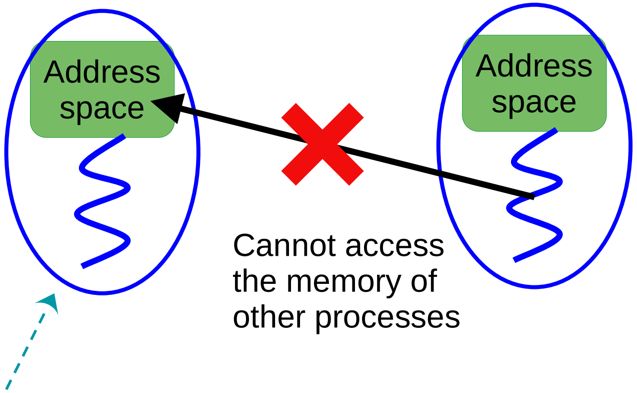
- Processes and Threads are two ways to exploit parallelism i.e. execute code on different cores at the same time
- There can be more processes/threads than CPU cores, but for HPC purpose, we usually use one threads per core

Processes ~ program

- Have their own address space (memory with variables)
- The process address space is not accessible to other processes
- Contain at least one thread

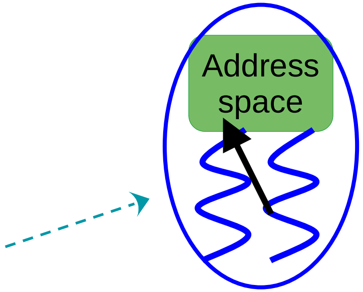
Threads ~ execution flow

- Use the address space of the process
- Threads within one process share the same address space
- Lightweight ~ Faster to create and destroy than processes



Cannot access the memory of other processes

Process with one thread



Process with two threads

With a process, threads share the same memory

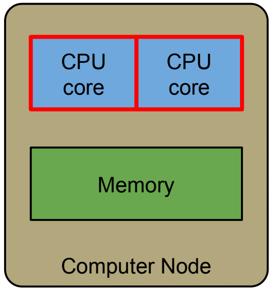
Memory Models for Parallel Programming

Shared Memory
Single Computing Node

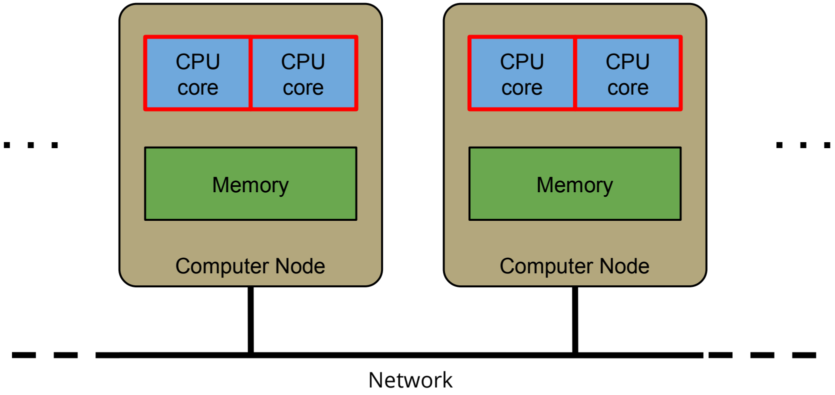
vs

Distributed Memory
Multiple Computing Nodes

That's your laptop or workstation!



That's an HPC cluster!



Memory Models for Parallel Programming

Shared Memory

Single Computing Node

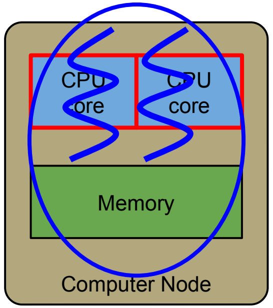
vs

Distributed Memory

Multiple Computing Nodes

That's your laptop or workstation!

One process with multiple threads



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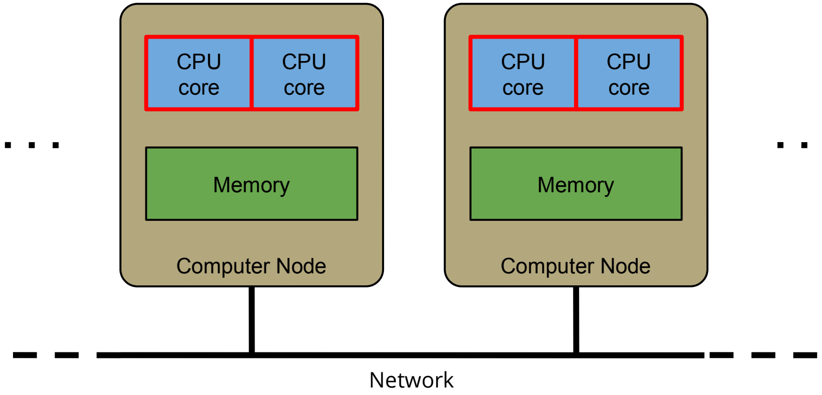


To use multiple CPUs on the same computing node

- Distribute the **computation**
- All threads share the same memory space
- Require synchronizations instead of communications

⇒ **OpenMP**: Open Multi-Processing

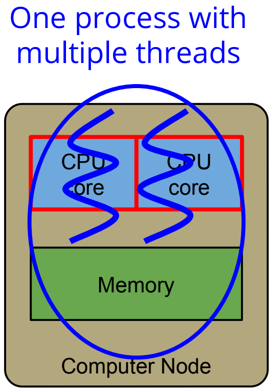
Memory Models for Parallel Programming

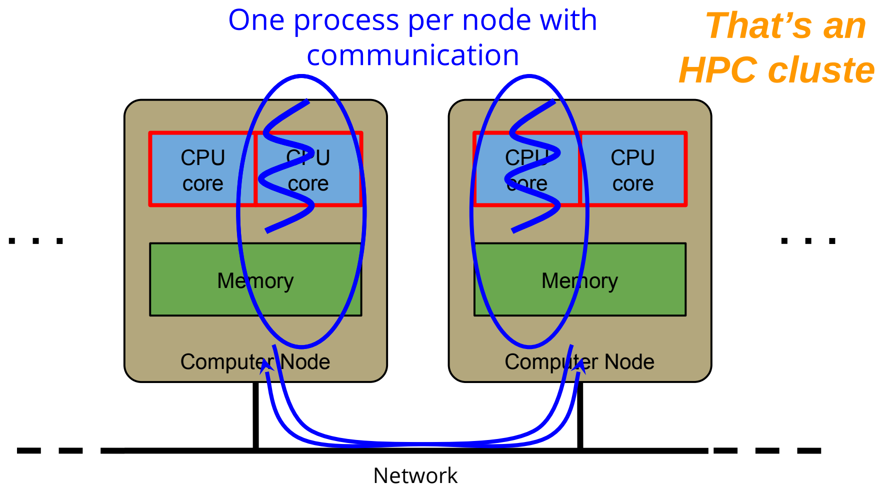
Shared Memory
Single Computing Node

vs

Distributed Memory
Multiple Computing Nodes

That's your laptop or workstation!





That's an HPC cluster!

To use multiple CPUs on the same computing node

- Distribute the **computation**
- All threads share the same memory space
- Require synchronizations instead of communications

⇒ **OpenMP**: Open Multi-Processing

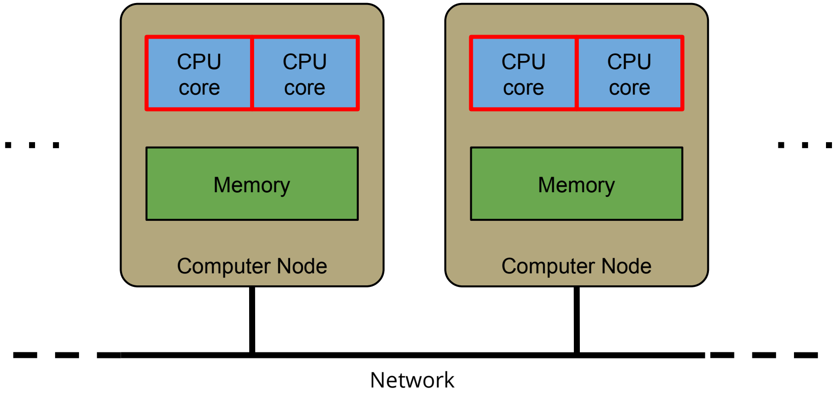
To use multiples CPUs on multiple computing nodes

- Distribute the **computation** and the **data**
- Processes cannot access the memory of others
- Exchange messages on the network

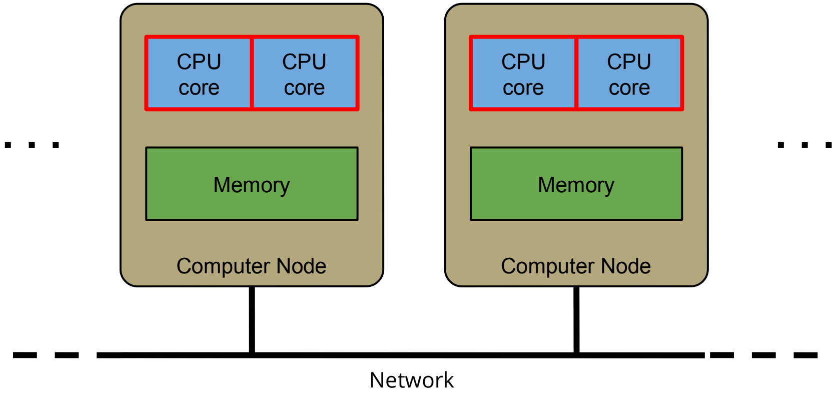
⇒ **MPI**: Message Passing Interface

Memory Models for Parallel Programming

Only Distributed Memory
All cores on Multiple Computing Nodes



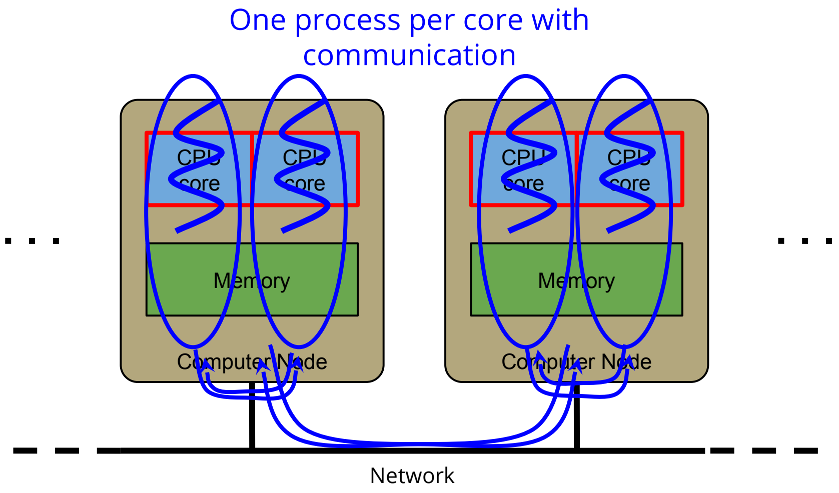
Hybrid Shared + Distributed Memory
All cores on Multiple Computing Nodes



Memory Models for Parallel Programming

Only Distributed Memory

All cores on Multiple Computing Nodes

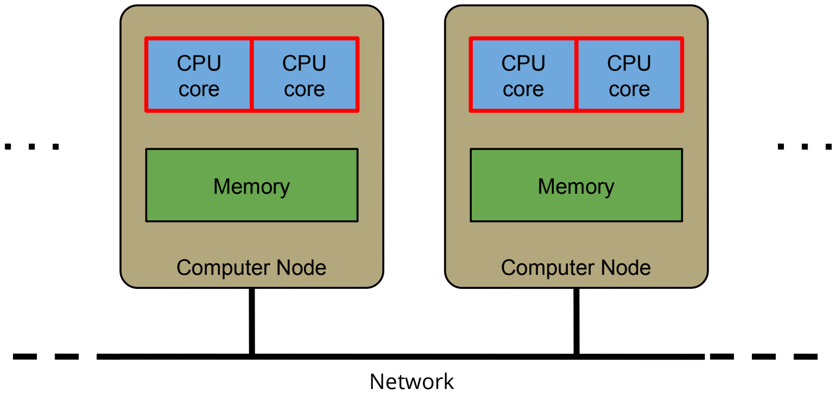


The processes cannot access the memory of others

- Use communication even within a node
- Communication within a node can be optimized by the software layer (e.g. memory copy instead to bypass the network)
- Simplify the programming ⇒ **MPI**

Hybrid Shared + Distributed Memory

All cores on Multiple Computing Nodes

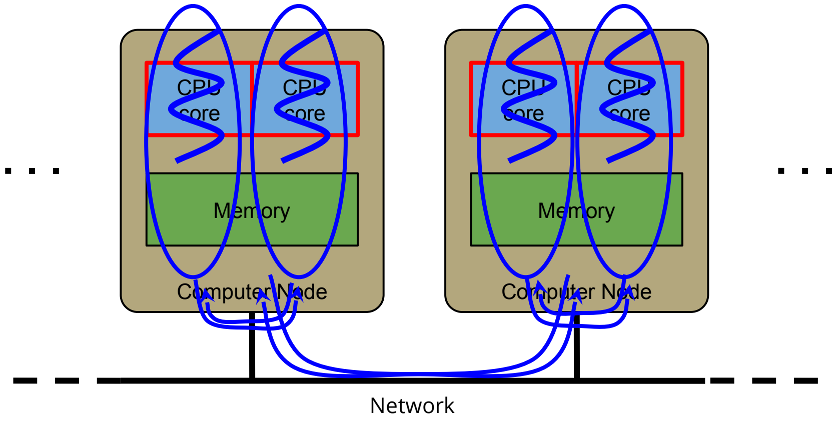


Memory Models for Parallel Programming

Only Distributed Memory

All cores on Multiple Computing Nodes

One process per core with communication



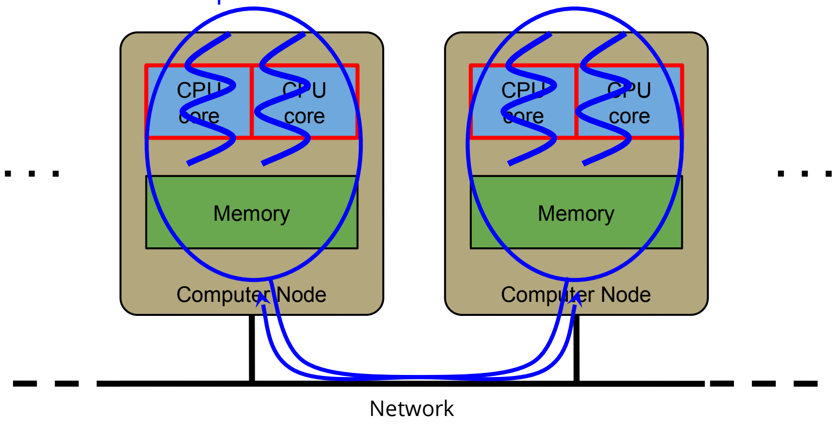
The processes cannot access the memory of others

- Use communication even within a node
- Communication within a node can be optimized by the software layer (e.g. memory copy instead to bypass the network)
- Simplify the programming ⇒ **MPI**

Hybrid Shared + Distributed Memory

All cores on Multiple Computing Nodes

One process per node with one thread per core and communication



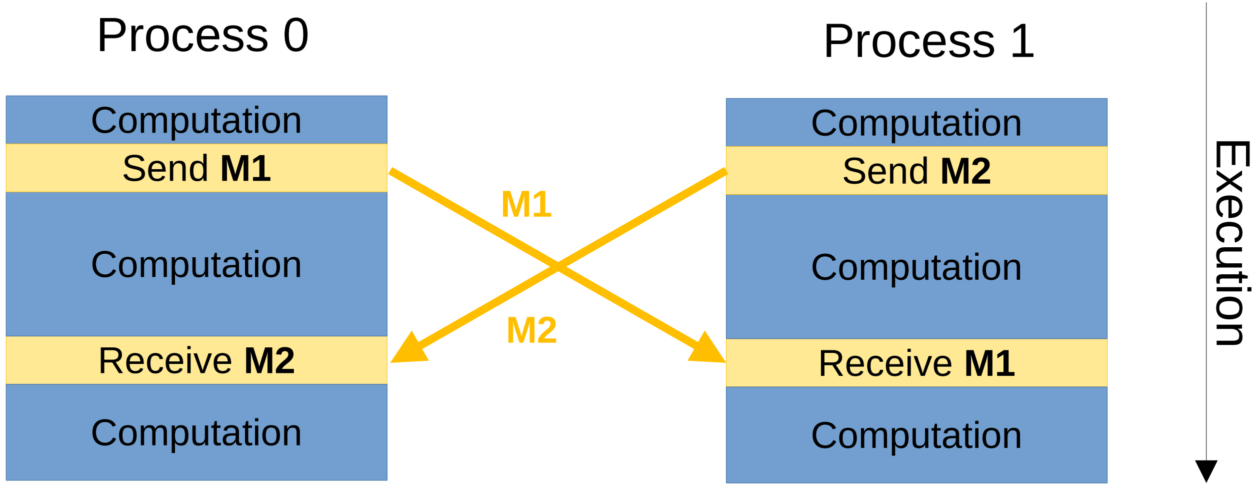
Use shared memory within a computing node and distributed memory across nodes

- To be adapted to the hardware
- Benefit of both models, but more complex

⇒ **Hybrid MPI + OpenMP**

Distributed Memory Programming with MPI

Message Passing Model: Multiple processes run in parallel and exchange messages
→ Analogy: Paper mails if your network is slow, E-mails if your network is fast



- **MPI is a standard**: MPI-1.0 in 1994, MPI-2.0 in 1997, MPI-3.0 in 2012, MPI-4.0 in 2021
- Different implementations: OpenMPI, MPICH, MVAPICH, Intel MPI, etc.
- Standard API in C and Fortran, non-official API in C++, Python

MPI Concepts

Fixed number of processes

- Specified at application startup, unchanged throughout execution

Communicator

- Abstraction for a group of processes that can communicate
- A process can belong to multiple communicators
- Default and global communicator: MPI_COMM_WORLD

Process Rank

- Index of a process within a communicator
- Used to identify other processes in communication operations

MPI Programming Interface

Lifecycle management

- `MPI_Init`, `MPI_Finalize`, `MPI_Abort`

Communicators

- `MPI_Comm_Size`, `MPI_Comm_Rank`
- `MPI_Comm_create`, `MPI_Comm_dup`, `MPI_Comm_join`

Datatype and Buffer

- `MPI_Type_*`
- `MPI_Pack`, `MPI_Unpack`

Blocking point-to-point

- `MPI_Send`, `MPI_Recv`

Non-blocking communications

- `MPI_Isend`, `MPI_Irecv`
- `MPI_Wait`, `MPI_Waitall`

Collective communications

- `MPI_Bcast`, `MPI_Reduce`, `MPI_Gather`, `MPI_Scatter`
- `MPI_Barrier`

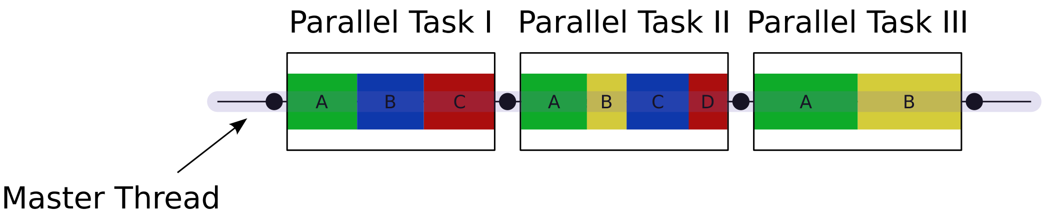
One-sided communications

- `MPI_Win_create`, `MPI_wait`
- `MPI_Put`, `MPI_Get`

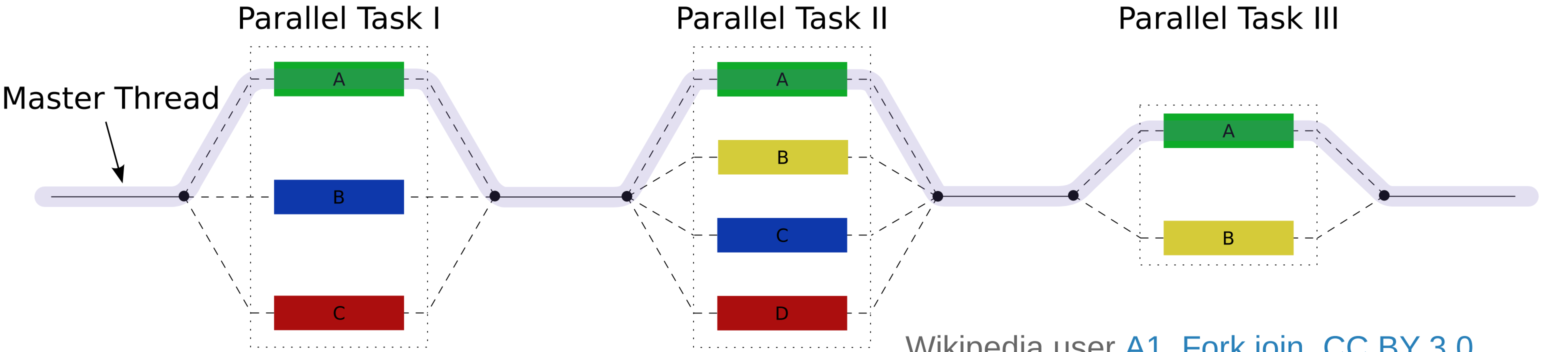
Shared Memory Multi-Processing with OpenMP

- OpenMP is based on the **Fork-Join** model

→ Analogy: Restaurant kitchen, the cooks share the utensils and ingredients to prepare the dishes



Threads are spawned dynamically in each parallel region



Wikipedia user A1, Fork join, CC BY 3.0

- Portable standard API for C, C++ and Fortran
- Support multi-cores and accelerators

OpenMP Concepts

Based on compiler directives **`#pragma omp ...`**

Example

```
#pragma omp parallel for
for (int i = 0; i < 100000; i++) {
    a[i] = 2 * i;
}
```

- Can control work distribution with the **schedule** clause (static, dynamic, guided)
- Threads can share variables, cf **private** or **shared** clauses
  → Caution with concurrent accesses!

In principle → Simple to use, minor modifications to the code

In practice → Might require changes in loops and data structures

Introduction to

High-Performance Computing

Parallel Programming Caveats

Race Condition 1/3

"Debugging programs containing race conditions is no fun at all."
Andrew S. Tanenbaum, *Modern Operating Systems*, 1992.

Race condition

- A **timing-dependent** error involving shared state
- It runs fine most of the time, and from time to time, something weird and unexplained appears

Race Condition 2/3

Code example

```
void deposit(Account* account, double amount)
{

  account->balance += amount;

}
```

Race Condition 2/3

Code example

```
void deposit(Account* account, double amount)
{
  READ balance
  ADD amount
  WRITE balance
}
```

Race Condition 2/3

Code example

```
void deposit(Account* account, double amount)
{
  READ balance
  ADD amount
  WRITE balance
}
```

Concurrent execution

Thread 1 calls `deposit(A,10)`   Thread 2 calls `deposit(A,1000)`

```
READ balance (0)
                                   READ balance (0)
                                   ADD 1000
                                   WRITE balance (1000)
ADD 10
WRITE balance (10)
```

Race Condition 2/3

Code example

```
void deposit(Account* account, double amount)
{
  READ balance
  ADD amount
  WRITE balance
}
```

Concurrent execution

```
Thread 1 calls deposit(A,10)              Thread 2 calls deposit(A,1000)
READ balance (0)

                                       READ balance (0)
                                       ADD 1000
                                       WRITE balance (1000)

ADD 10
WRITE balance (10)
```

Race Condition 2/3

Code example

```
void deposit(Account* account, double amount)
{
  READ balance
  ADD amount
  WRITE balance
}
```

Concurrent execution

Thread 1 calls `deposit(A,10)`	Thread 2 calls `deposit(A,1000)`
`READ balance (0)`	
	`READ balance (0)`
	`ADD 1000`
	`WRITE balance (1000)`
`ADD 10`	
`WRITE balance (10)`	

Race Condition 2/3

Code example

```
void deposit(Account* account, double amount)
{
  READ balance
  ADD amount
  WRITE balance
}
```

Concurrent execution

```
Thread 1 calls deposit(A,10)                     Thread 2 calls deposit(A,1000)
READ balance (0)

                                             READ balance (0)
                                             ADD 1000
                                             WRITE balance (1000)
ADD 10
WRITE balance (10)
```

Race Condition 2/3

Code example

```
void deposit(Account* account, double amount)
{
  READ balance
  ADD amount
  WRITE balance
}
```

Concurrent execution

```
Thread 1 calls deposit(A,10)                  Thread 2 calls deposit(A,1000)
READ balance (0)

                                          READ balance (0)
                                          ADD 1000
                                          WRITE balance (1000)

ADD 10
WRITE balance (10)
```

Race Condition 2/3

Code example

```
void deposit(Account* account, double amount)
{
  READ balance
  ADD amount
  WRITE balance
}
```

Concurrent execution

Thread 1 calls `deposit(A,10)`　　　　Thread 2 calls `deposit(A,1000)`

```
READ balance (0)

                                     READ balance (0)
                                     ADD 1000
                                     WRITE balance (1000)

ADD 10
WRITE balance (10)
```

Race Condition 2/3

Code example

```
void deposit(Account* account, double amount)
{
  READ balance
  ADD amount
  WRITE balance
}
```

Concurrent execution

```
Thread 1 calls deposit(A,10)              Thread 2 calls deposit(A,1000)
READ balance (0)

                                      READ balance (0)
                                      ADD 1000
                                      WRITE balance (1000)

ADD 10
WRITE balance (10)
```

Race Condition 2/3

Code example

```
void deposit(Account* account, double amount)
{
  READ balance
  ADD amount
  WRITE balance
}
```

Concurrent execution

```
Thread 1 calls deposit(A,10)            Thread 2 calls deposit(A,1000)
READ balance (0)

                                     READ balance (0)
                                     ADD 1000
                                     WRITE balance (1000)
ADD 10
WRITE balance (10)
```

→ **Result: balance is 10 instead of 1010**

Without protection, any interleave combination is possible!

Race Condition 3/3

Different kind of race conditions

- **Data race**: Concurrent accesses to a shared variable
- **Atomicity bugs**: Code does not enforce the atomicity for a group of memory accesses, e.g. *Time of check to time of use*
- **Order bugs**: Operations are not executed in order
  Compilers and processors can actually re-order instructions

What to do?

- Protect critical sections: **Mutexes**, **Semaphores**, etc.
- Use atomic instructions and memory barriers (low level)
- Use compiler builtin for atomic operations (higher level)

Deadlock 1/3

Deadlock, photograph by David Maitland

"I would love to have seen them go their separate ways, but I was exhausted. The frog was all the time trying to pull the snake off, but the snake just wouldn't let go."

Deadlock 2/3

Code Example

```
void deposit(Account* account,
             double amount)
{
  lock(account->mutex);
  account->balance += amount;
  unlock(account->mutex);
}
```

```
void transfer(Account* accA,
              Account* accB,
              double amount)
{
  lock(accA->mutex);
  lock(accB->mutex);
  accA->balance += amount;
  accB->balance -= amount;
  unlock(accA->mutex);
  unlock(accB->mutex);
}
```

→ Use mutexes (lock/unlock) to protect concurrent accesses?

Deadlock 3/3

Concurrent Execution

Thread 1 calls `transfer(A,B,10)`

```
lock(A->mutex);

lock(B->mutex); // wait until
                // B is unlocked



...
```

Thread 2 calls `transfer(B,A,20)`

```

lock(B->mutex);



lock(A->mutex); // wait until
                // A is unlocked
...
```

Deadlock 3/3

Concurrent Execution

Thread 1 calls `transfer(A,B,10)`

```
lock(A->mutex);

lock(B->mutex); // wait until
                // B is unlocked

...
```

Thread 2 calls `transfer(B,A,20)`

```
lock(B->mutex);

lock(A->mutex); // wait until
                // A is unlocked
...
```

Deadlock 3/3

Concurrent Execution

Thread 1 calls `transfer(A,B,10)`

```
lock(A->mutex);

lock(B->mutex); // wait until
                // B is unlocked

...
```

Thread 2 calls `transfer(B,A,20)`

```
lock(B->mutex);

lock(A->mutex); // wait until
                // A is unlocked

...
```

Deadlock 3/3

Concurrent Execution

Thread 1 calls `transfer(A,B,10)`

```
lock(A->mutex);

lock(B->mutex); // wait until
                // B is unlocked


...
```

Thread 2 calls `transfer(B,A,20)`

```

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Thread 1 calls `transfer(A,B,10)`

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→ We have a deadlock!

Thread 2 calls `transfer(B,A,20)`

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...
```

Deadlock 3/3

Concurrent Execution

Thread 1 calls `transfer(A,B,10)`

```
lock(A->mutex);

lock(B->mutex); // wait until
                // B is unlocked



...
```

→ **We have a deadlock!**

Thread 2 calls `transfer(B,A,20)`

```

lock(B->mutex);


lock(A->mutex); // wait until
                // A is unlocked
...
```

What to do?

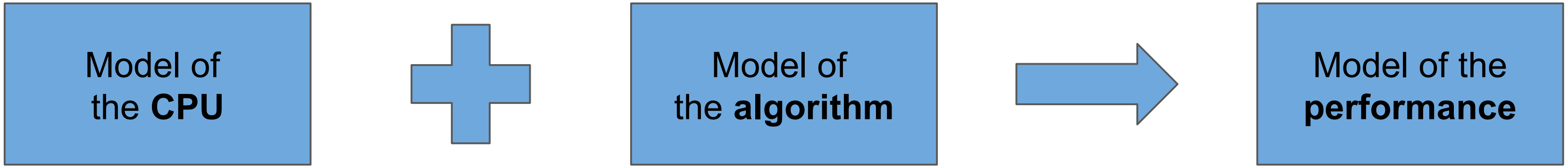
- Think before writing multithread code
- Use high level programming model: OpenMP, Intel TBB, MPI, etc.
- Theoretical analysis
- Software for thread safety analysis

Introduction to

High-Performance Computing

Performance Modeling and Analysis

Performance Modeling of a CPU → Roofline Model



Model of the **CPU**

Model of the **algorithm**

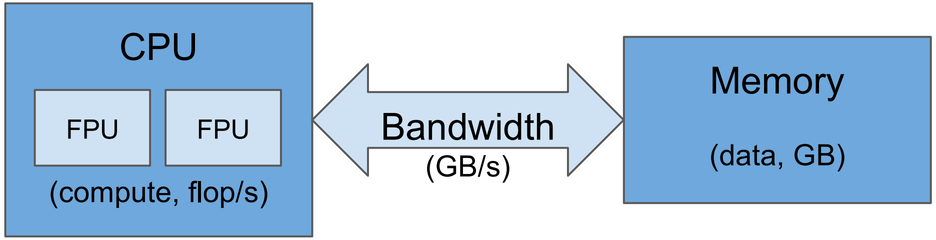
Model of the **performance**

- Estimate the **performance** of an **algorithm** on a given **CPU**
    - Also applies to GPUs, TPUs, etc.
- Throughput oriented model
- Identify the bottleneck
- Allow to improve the implementation of an algorithm

Roofline model

Roofline model

Model of a CPU

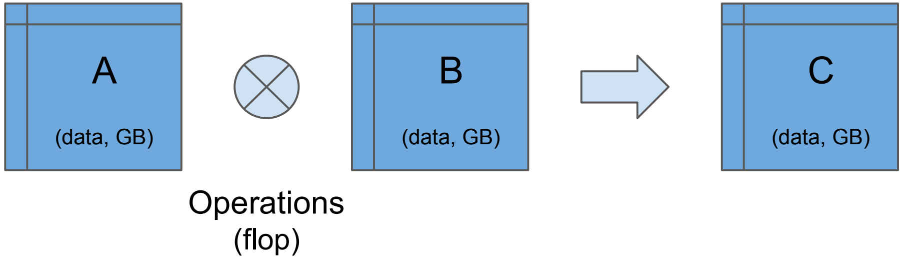


Peak performance limited by

- Compute operations: Gflop/s
- Data bandwidth: GB/s

Roofline model

Model of an algorithm



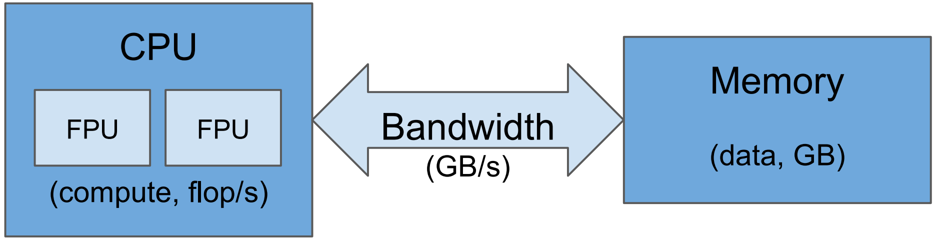
Algorithm characteristics

- Operations: Gflop
- Data: GB

Arithmetic Intensity

AI: flop / Byte

Model of a CPU



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Roofline model

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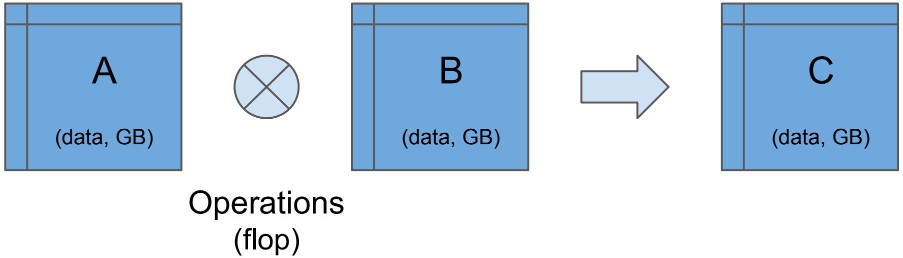

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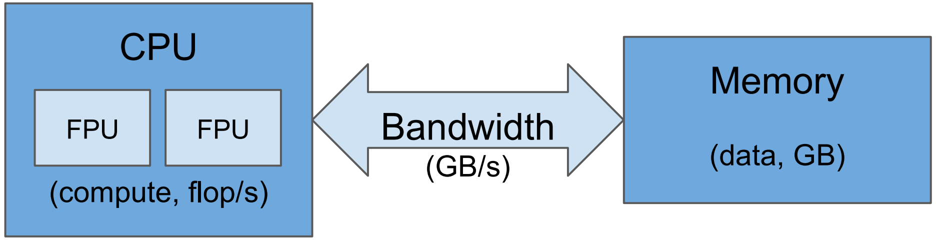


Peak performance limited by

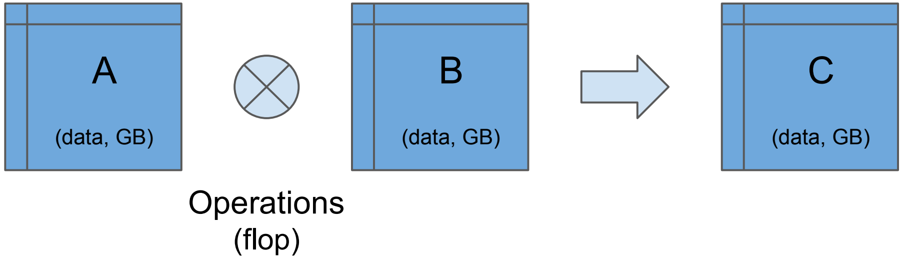
- Compute operations: Gflop/s
- Data bandwidth: GB/s

Attainable performance

$$\text{Gflop/s} = \min \begin{cases} \text{Peak Gflop/s} \\ \text{AI x Peak GB/s} \end{cases}$$

Roofline model

Model of an algorithm



Algorithm characteristics

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Arithmetic Intensity

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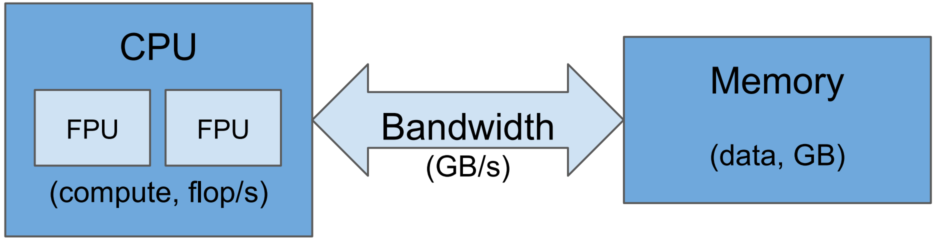
Model of a CPU



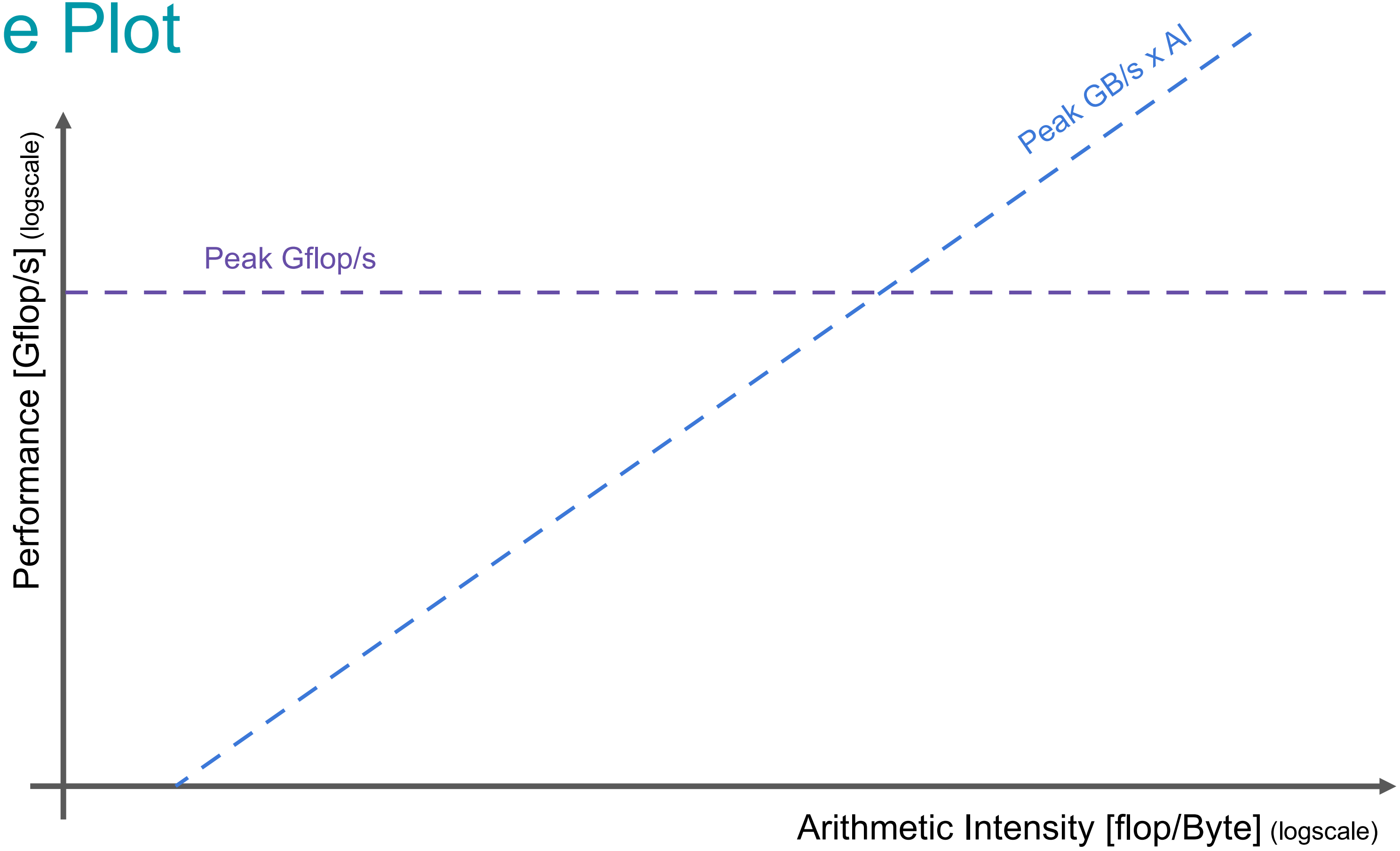
Peak performance limited by

- Compute operations: Gflop/s
- Data bandwidth: GB/s

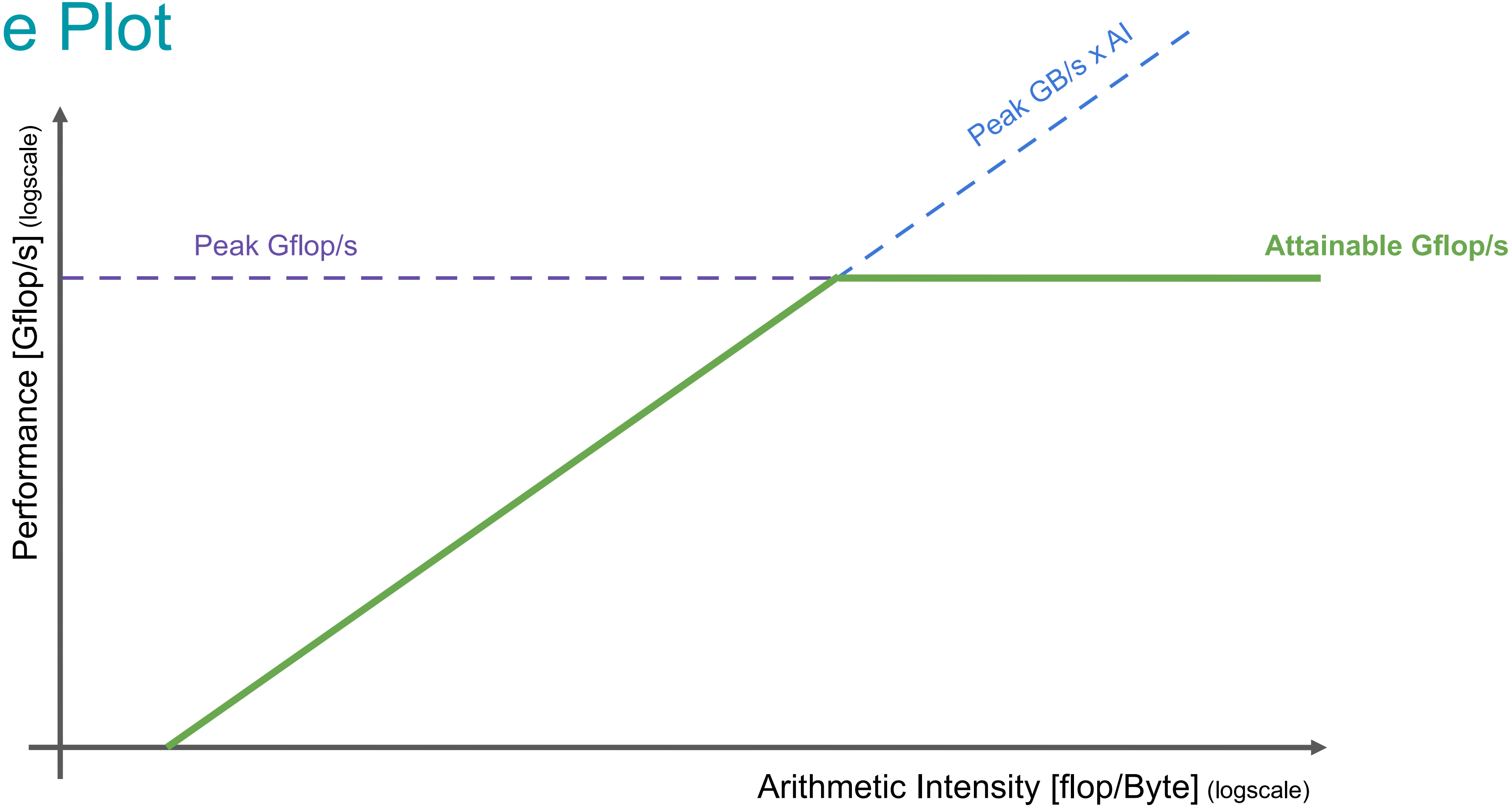
Attainable performance

$$\text{Gflop/s} = \min \begin{cases} \text{Peak Gflop/s} \\ \text{AI} \times \text{Peak GB/s} \end{cases}$$

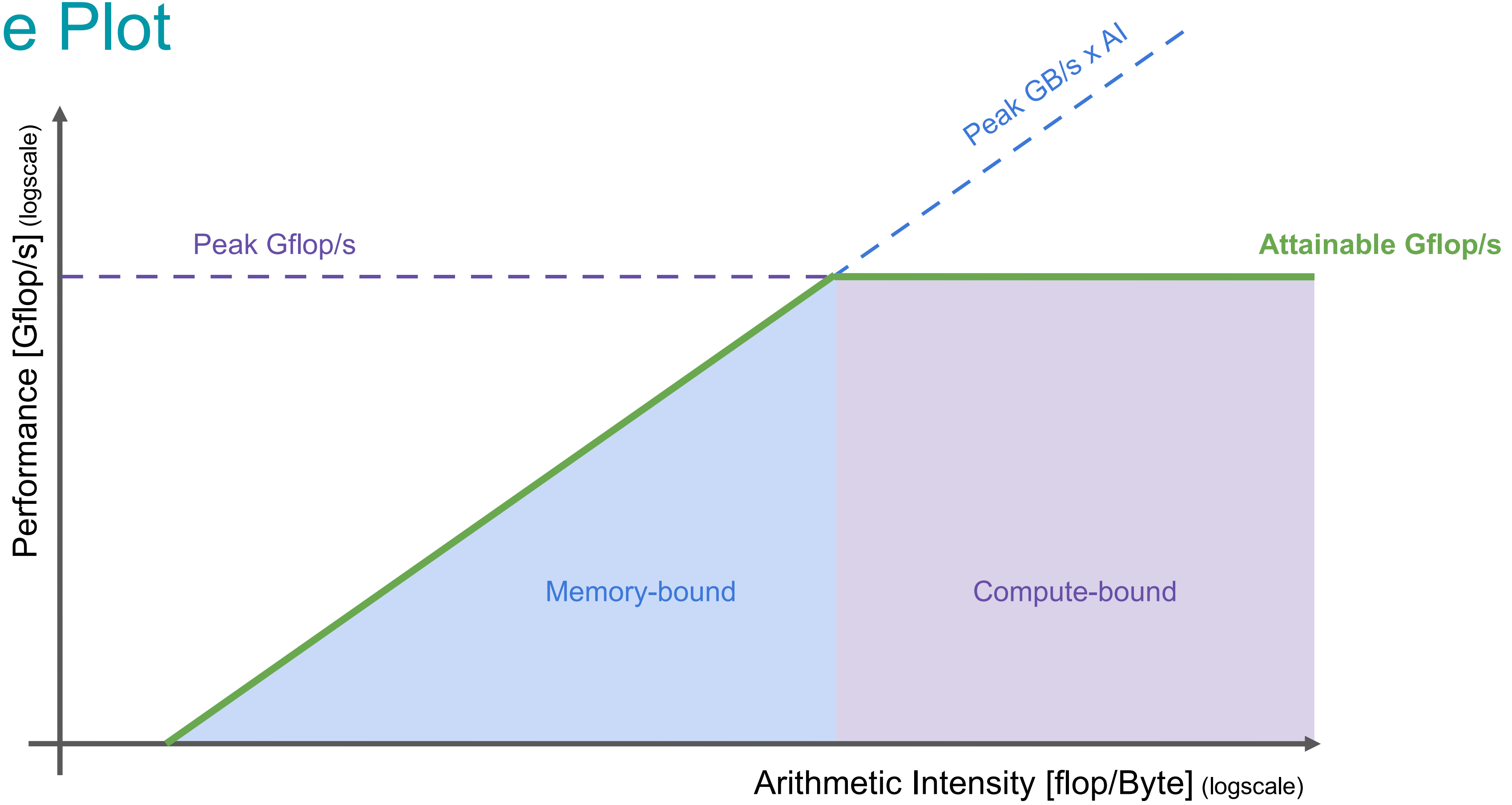
Roofline Plot



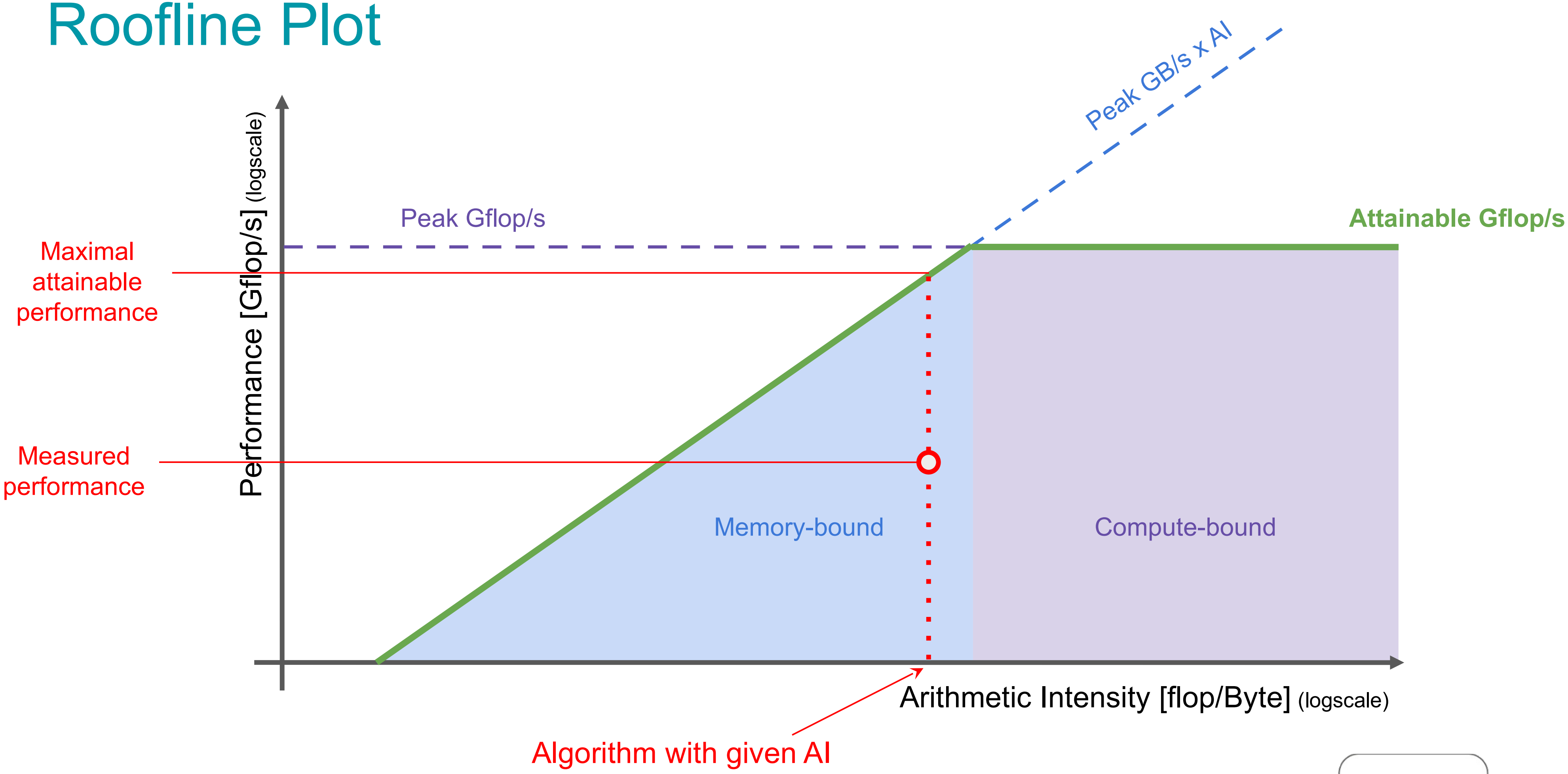
Roofline Plot


Peak GB/s x AI
Peak Gflop/s
Attainable Gflop/s
Performance [Gflop/s] (logscale)
Arithmetic Intensity [flop/Byte] (logscale)

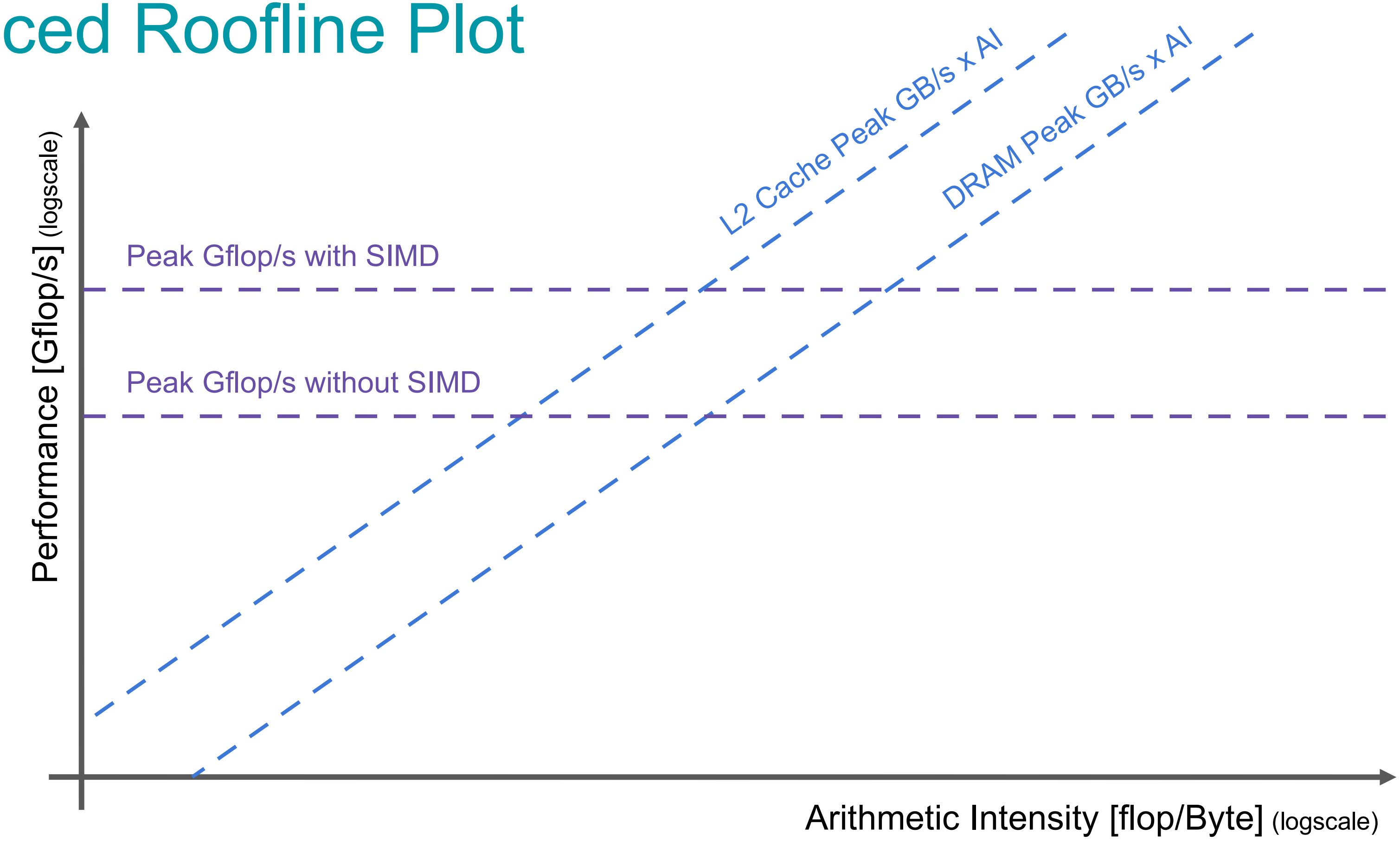
Roofline Plot


Peak GB/s x AI
Peak Gflop/s
Attainable Gflop/s
Performance [Gflop/s] (logscale)
Memory-bound
Compute-bound
Arithmetic Intensity [flop/Byte] (logscale)

Roofline Plot

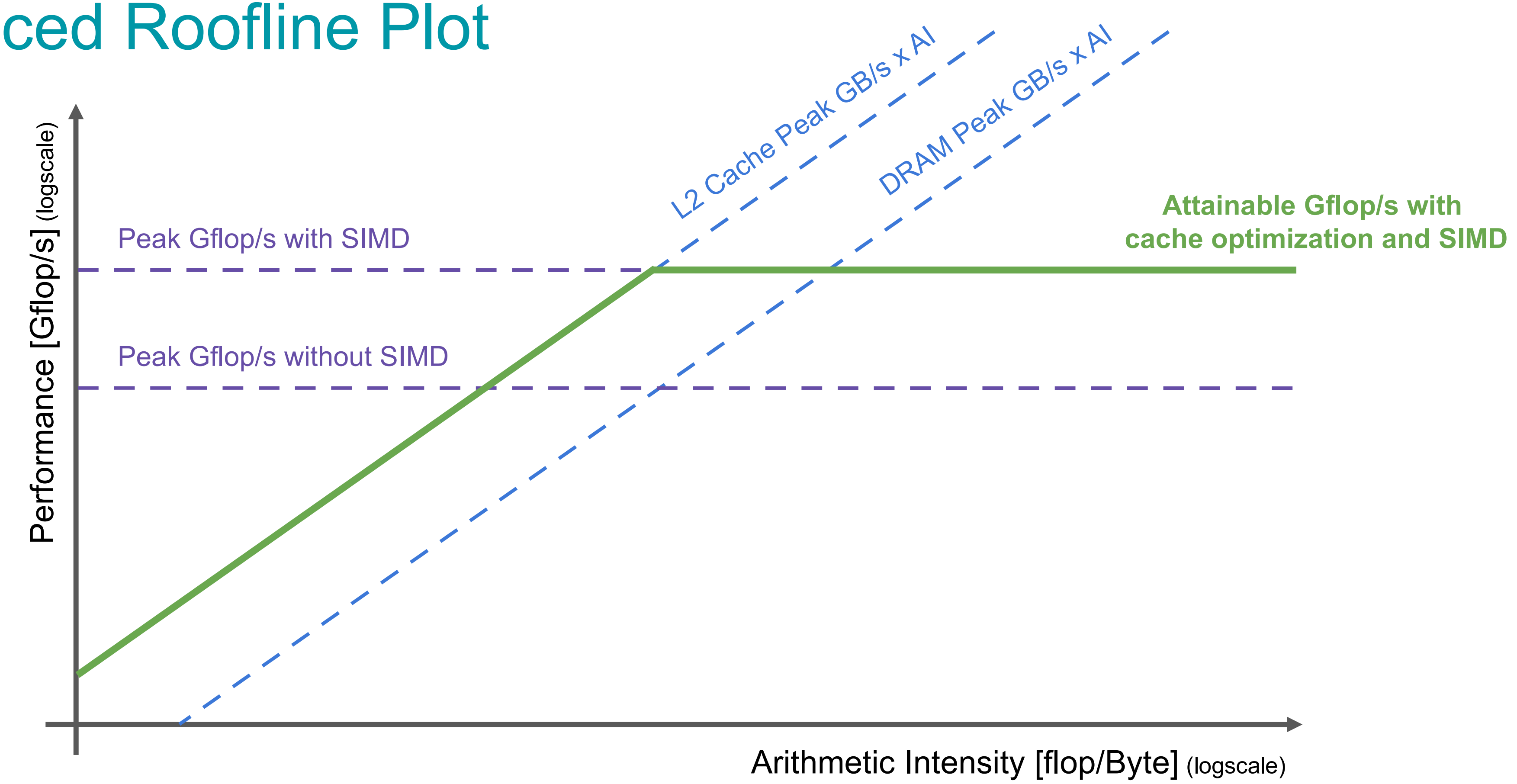


Advanced Roofline Plot


L2 Cache Peak GB/s x AI
DRAM Peak GB/s x AI
Peak Gflop/s with SIMD
Peak Gflop/s without SIMD
Performance [Gflop/s] (logscale)
Arithmetic Intensity [flop/Byte] (logscale)

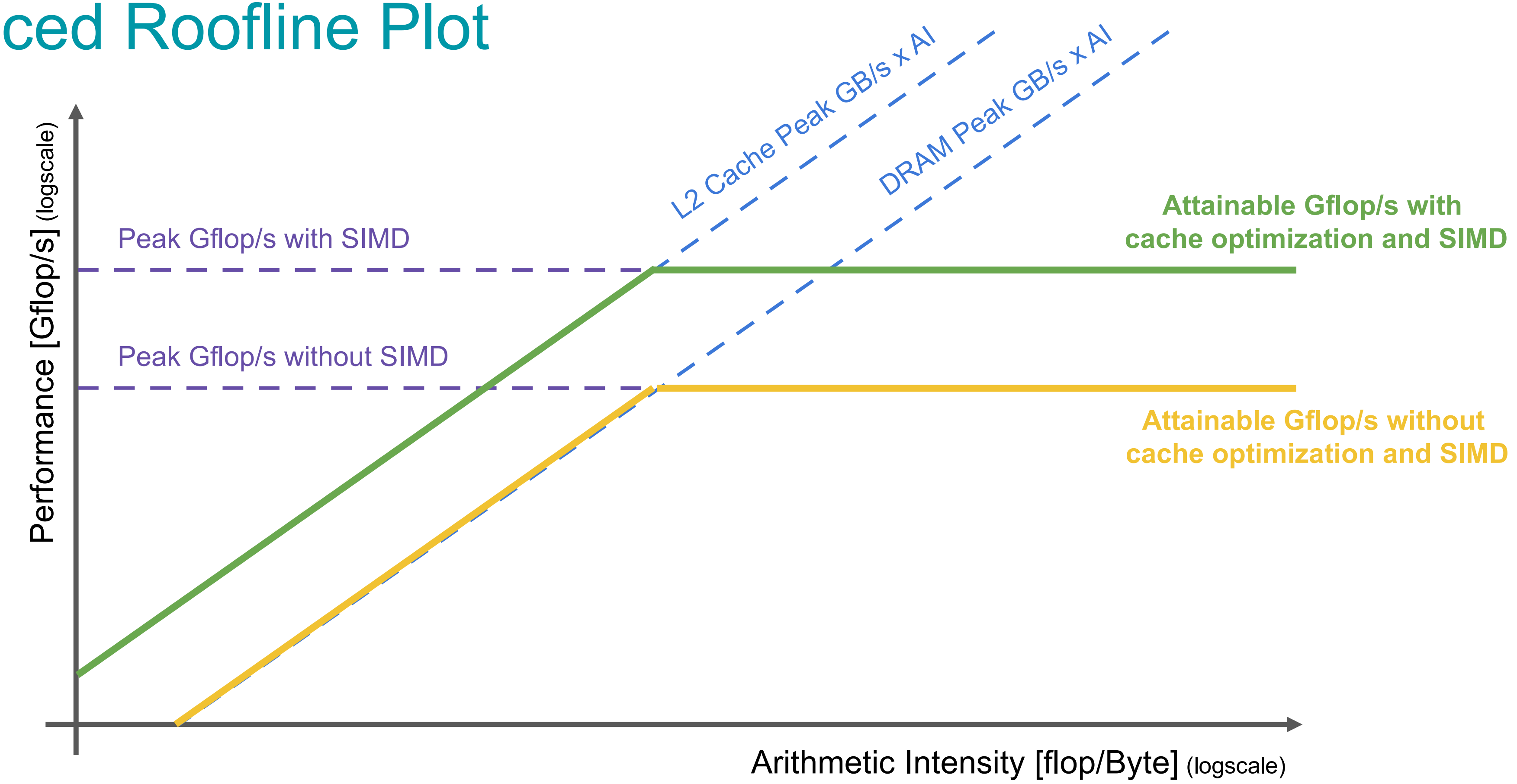
SIMD = Single Instruction, Multiple Data, ie vectorized instructions

Advanced Roofline Plot


L2 Cache Peak GB/s x AI
DRAM Peak GB/s x AI
Attainable Gflop/s with cache optimization and SIMD
Peak Gflop/s with SIMD
Peak Gflop/s without SIMD
Performance [Gflop/s] (logscale)
Arithmetic Intensity [flop/Byte] (logscale)

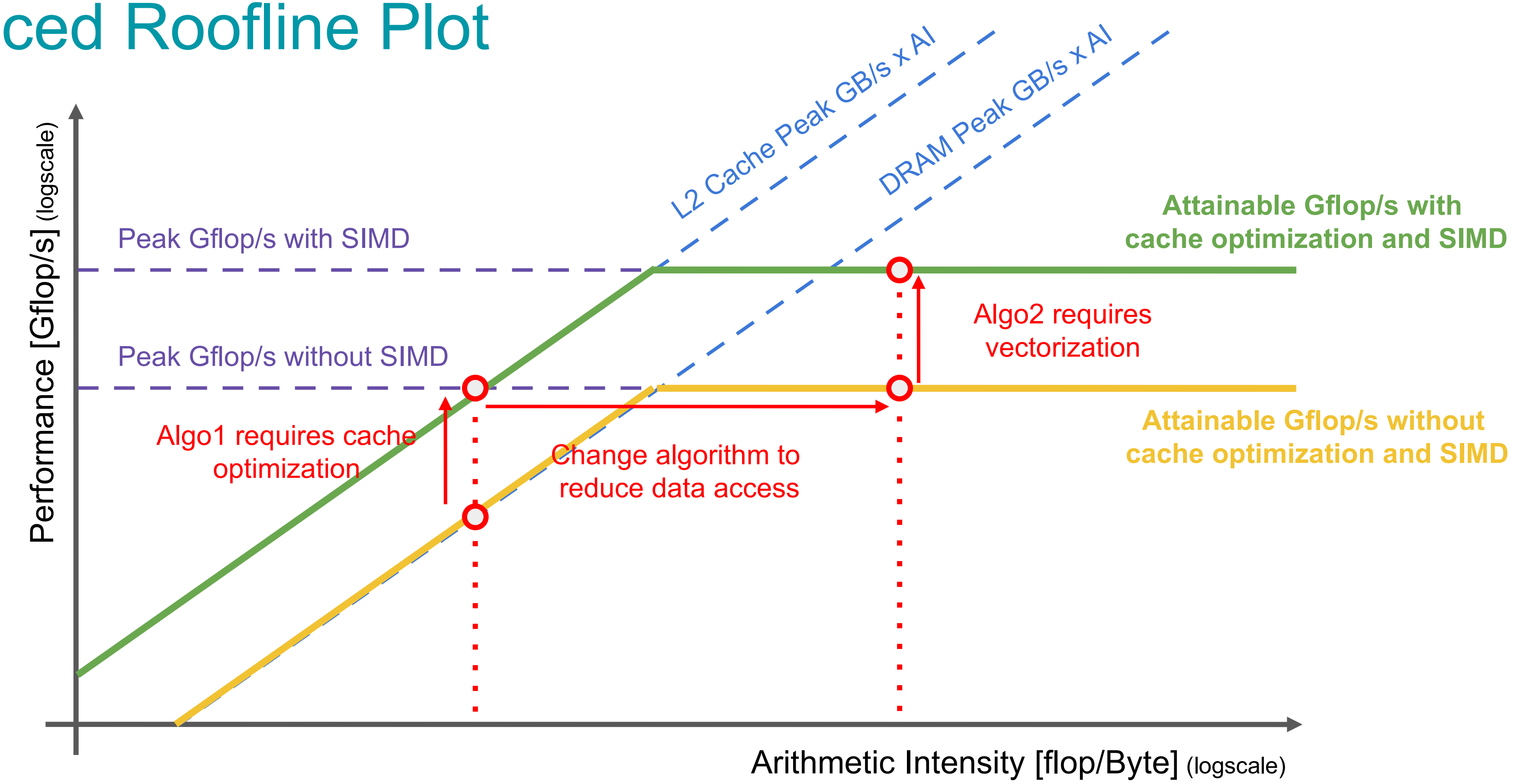
SIMD = Single Instruction, Multiple Data, ie vectorized instructions

Advanced Roofline Plot



SIMD = Single Instruction, Multiple Data, ie vectorized instructions

Advanced Roofline Plot


L2 Cache Peak GB/s x AI
DRAM Peak GB/s x AI
Attainable Gflop/s with cache optimization and SIMD
Peak Gflop/s with SIMD
Peak Gflop/s without SIMD
Algo2 requires vectorization
Algo1 requires cache optimization
Change algorithm to reduce data access
Attainable Gflop/s without cache optimization and SIMD
Performance [Gflop/s] (logscale)
Arithmetic Intensity [flop/Byte] (logscale)

SIMD = Single Instruction, Multiple Data, ie vectorized instructions

Comments about the Roofline Model

In theory

- Gives good insight of the bottleneck of a given algorithm

In practice, use automatic tools

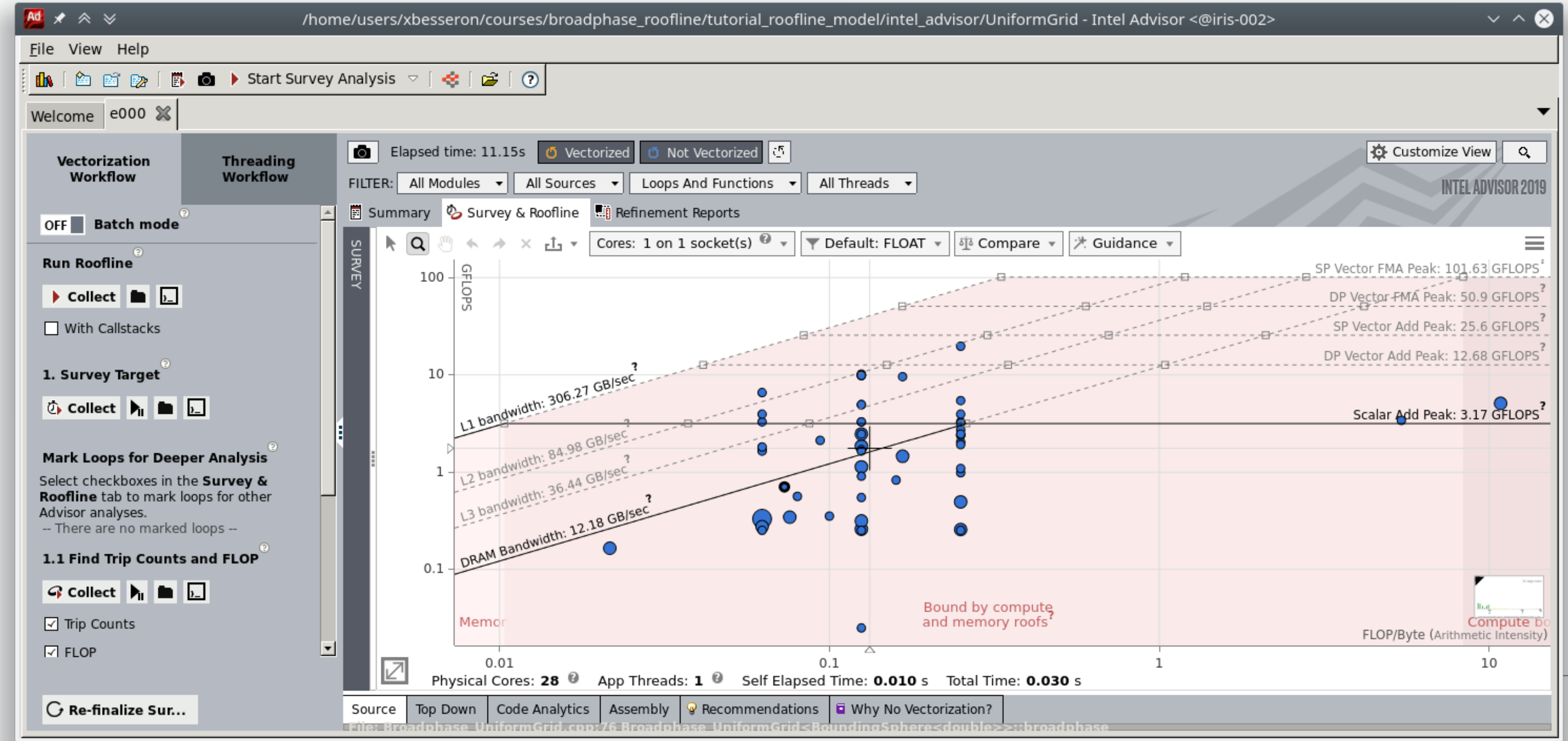
- CPU model can be hard to find
- Algorithm characterization is hard for complex algorithms

Warning

- The Roofline Model tells if an algorithm performs well,
- not if the algorithm is the best for your problem
- e.g. Bubble sort $O(n^2)$ vs Quicksort $O(n \log n)$

Roofline Model in practice

Example with Intel Advisor



/home/users/xbesseron/courses/broadphase_roofline/tutorial_roofline_model/intel_advisor/UniformGrid - Intel Advisor <@iris-002>

Elapsed time: 11.15s

FILTER: All Modules, All Sources, Loops And Functions, All Threads

Cores: 1 on 1 socket(s)

Default: FLOAT

OFF Batch mode

□ With Callstacks

Select checkboxes in the **Survey & Roofline** tab to mark loops for other Advisor analyses.

-- There are no marked loops --

☑ Trip Counts

☑ FLOP

Physical Cores: **28** App Threads: **1** Self Elapsed Time: **0.010** s Total Time: **0.030** s

File: Broadphase_UniformGrid.cpp:76 Broadphase_UniformGrid<BoundingSphere<double>>::broadphase

File View Help
Start Survey Analysis
Welcome
e000
Vectorization Workflow
Threading Workflow
Run Roofline
Collect
1. Survey Target
Collect
Mark Loops for Deeper Analysis
1.1 Find Trip Counts and FLOP
Collect
Re-finalize Sur...
Vectorized
Not Vectorized
Customize View
INTEL ADVISOR 2019
Summary
Survey & Roofline
Refinement Reports
SURVEY
Compare
Guidance
GFLOPS
100
10
1
0.1
SP Vector FMA Peak: 101.63 GFLOPS
DP Vector FMA Peak: 50.9 GFLOPS
SP Vector Add Peak: 25.6 GFLOPS
DP Vector Add Peak: 12.68 GFLOPS
Scalar Add Peak: 3.17 GFLOPS
L1 bandwidth: 306.27 GB/sec
L2 bandwidth: 84.98 GB/sec
L3 bandwidth: 36.44 GB/sec
DRAM Bandwidth: 12.18 GB/sec
Memor
Bound by compute and memory roofs
Compute bo
FLOP/Byte (Arithmetic Intensity)
0.01
0.1
1
10
Source
Top Down
Code Analytics
Assembly
Recommendations
Why No Vectorization?

Measuring Parallel Performance: Speedup and Scalability

- Number of processors → N
- Sequential Time → T_1
- Parallel Time → T_N

$$\text{Speedup} = \frac{T_1}{T_N}$$

$$\text{Efficiency} = \frac{\text{Speedup}}{N}$$

Strong Scalability:
Problem size is fixed, increase the number of processors
→ Constant amount of work in the study

Weak Scalability:
Increase the problem size and the nb of processors with the same ratio
→ Constant amount of work per processor

Measuring Parallel Performance: Speedup and Scalability

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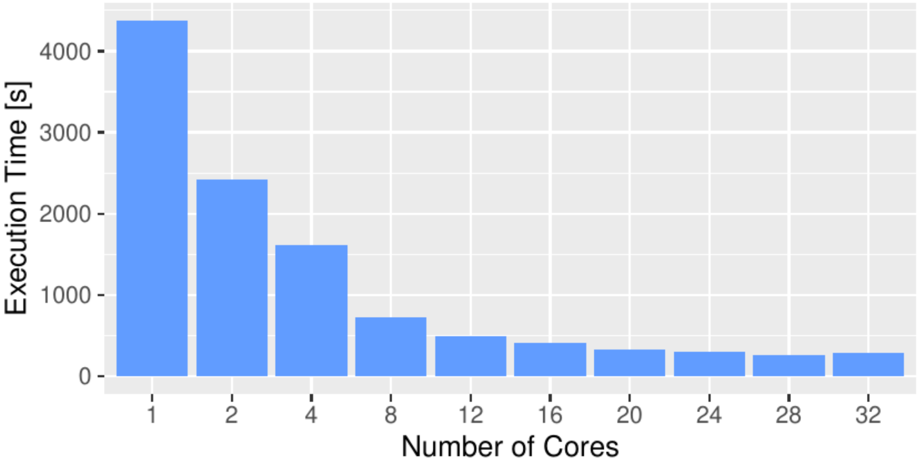
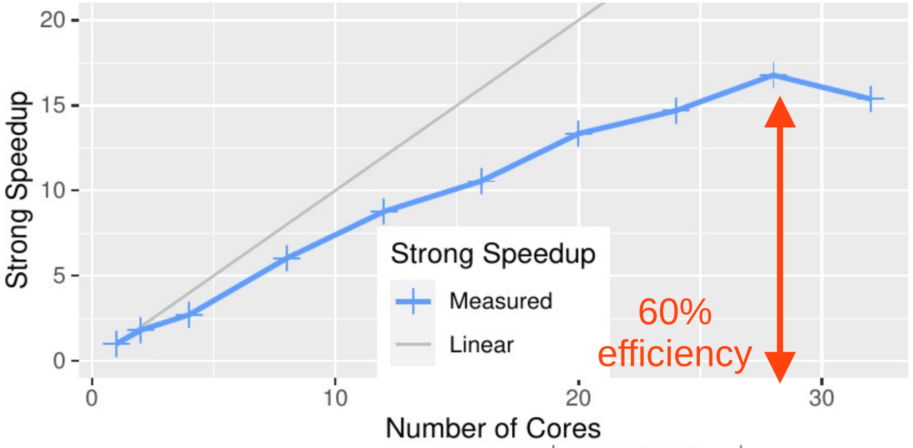
Strong scalability





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Weak Scalability:
Increase the problem size and the nb of processors with the same ratio
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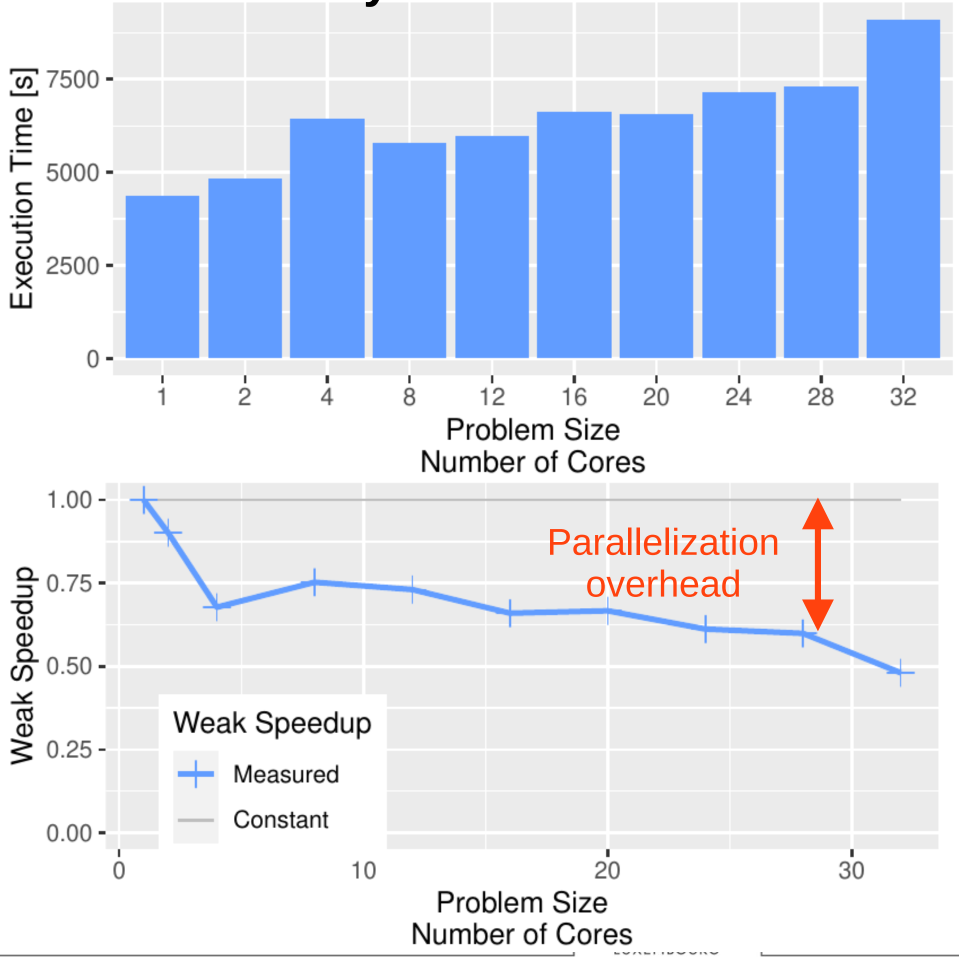
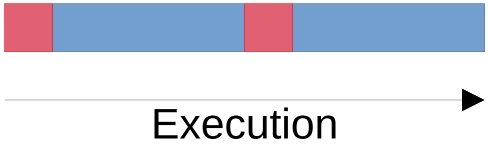
Weak scalability



Limit to Scalability: Amdahl’s law

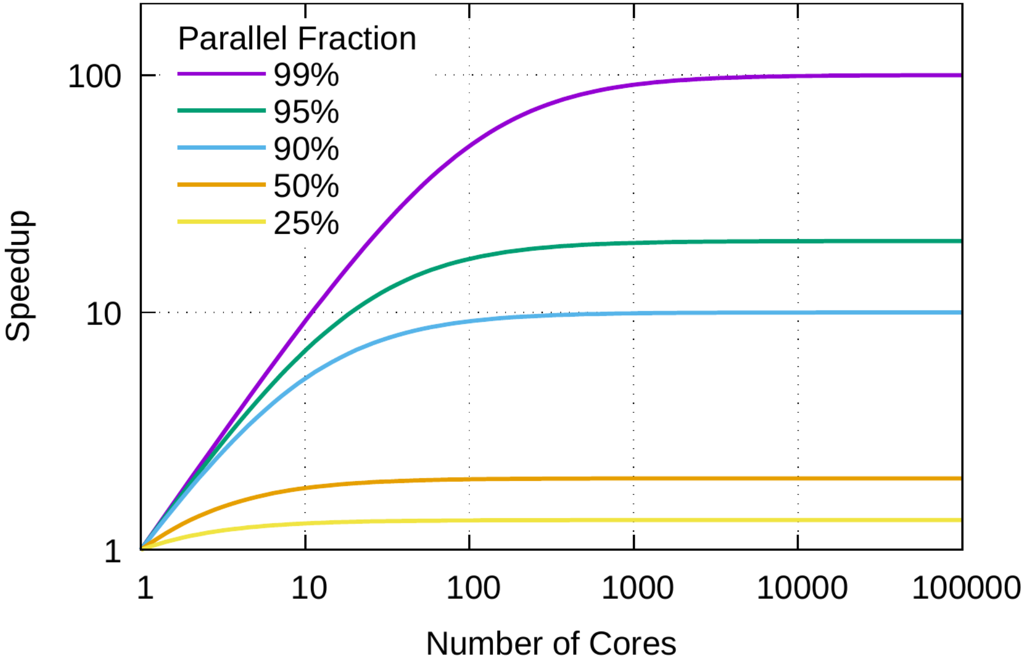
Amdahl’s law is a performance model



- Parallel fraction 🟦 → p
- Serial fraction 🟥 → 1 – p
- Number of processors → N

$$\text{Speedup} = \frac{T_1}{T_N} = \frac{1}{1 - p + \frac{p}{N}} \leqslant \frac{1}{1 - p}$$

Another performance model → Gustafson’s law



According to Amdahl’s law, scalability is bounded

Limit to Scalability: Load-balancing

Load-balancing

→ **Distribution of work between processors**

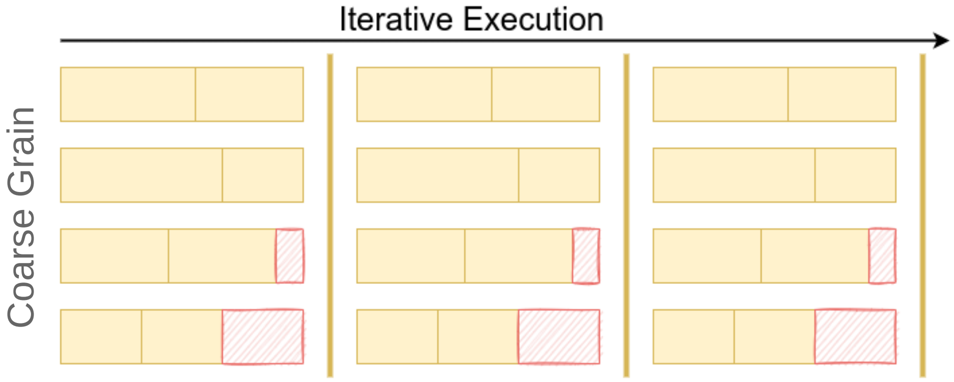
Load unbalance

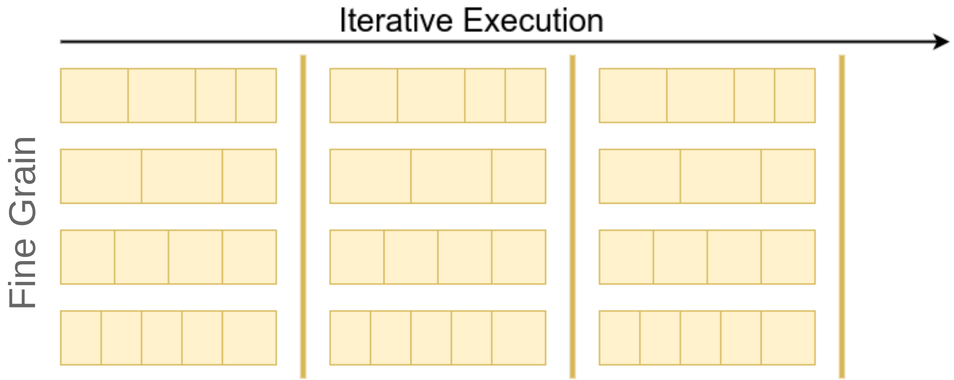
- Lost computation time
- Accumulates over iterations

→ **Limits the scalability**

- Coarse grain is more difficult to balance than fine grain
- Larger scale requires fine grain

→ A good estimation of the work of each task is critical





High-Performance Computing

for the **Simulation of Particles**

Discrete Element Method and XDEM

What is XDEM?

eXtended
Discrete
Element
Method

Simulation software for

Particles Dynamics

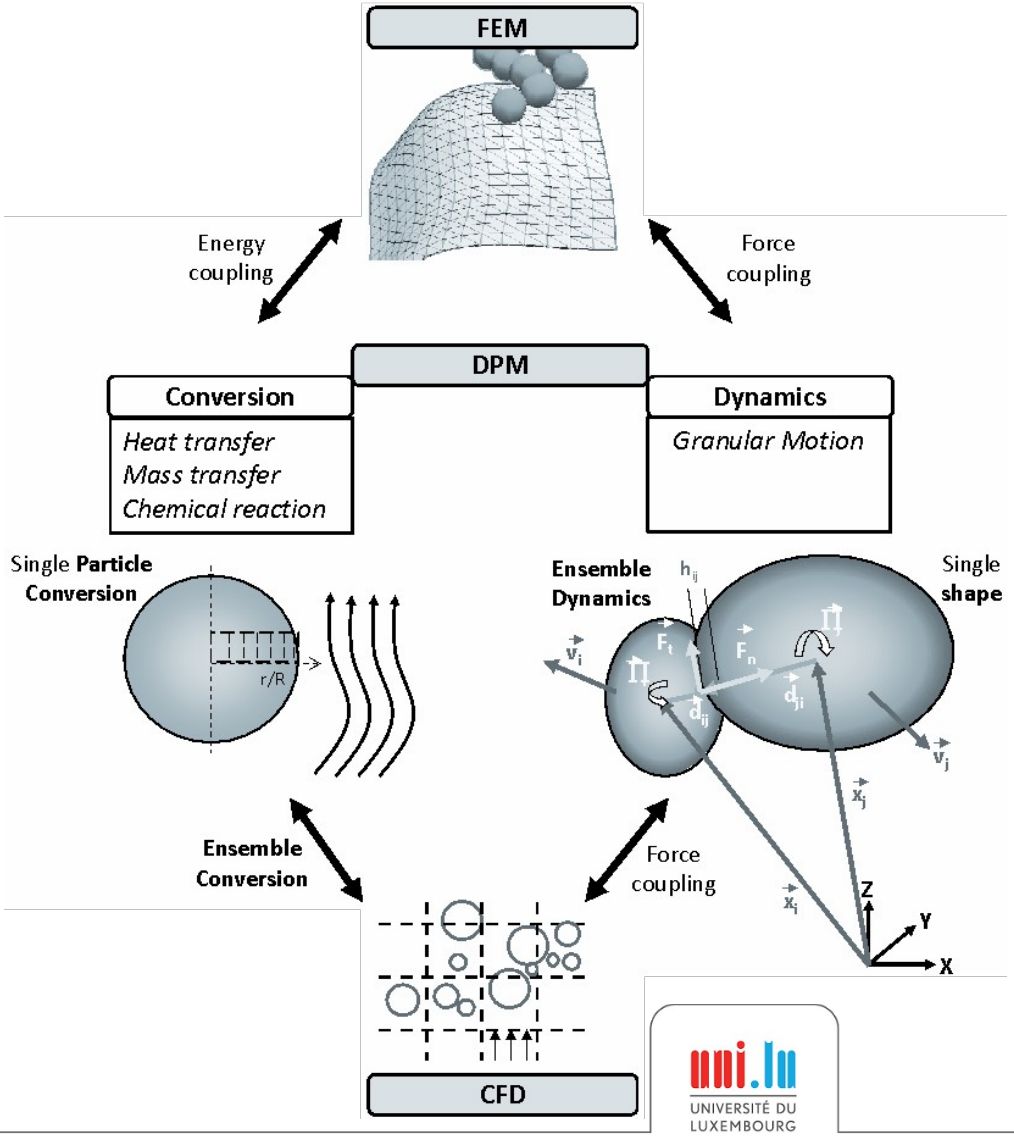
- Force and torques
- Particle motion

Particles Conversion

- Heat and mass transfer
- Chemical reactions

Coupled with

- Computational Fluid Dynamics (CFD)
- Finite Element Method (FEM)



https://luxdem.uni.lu/software/

What is XDEM?

eXtended Discrete Element Method

Simulation software for

Particles Dynamics

- Force and torques
- Particle motion

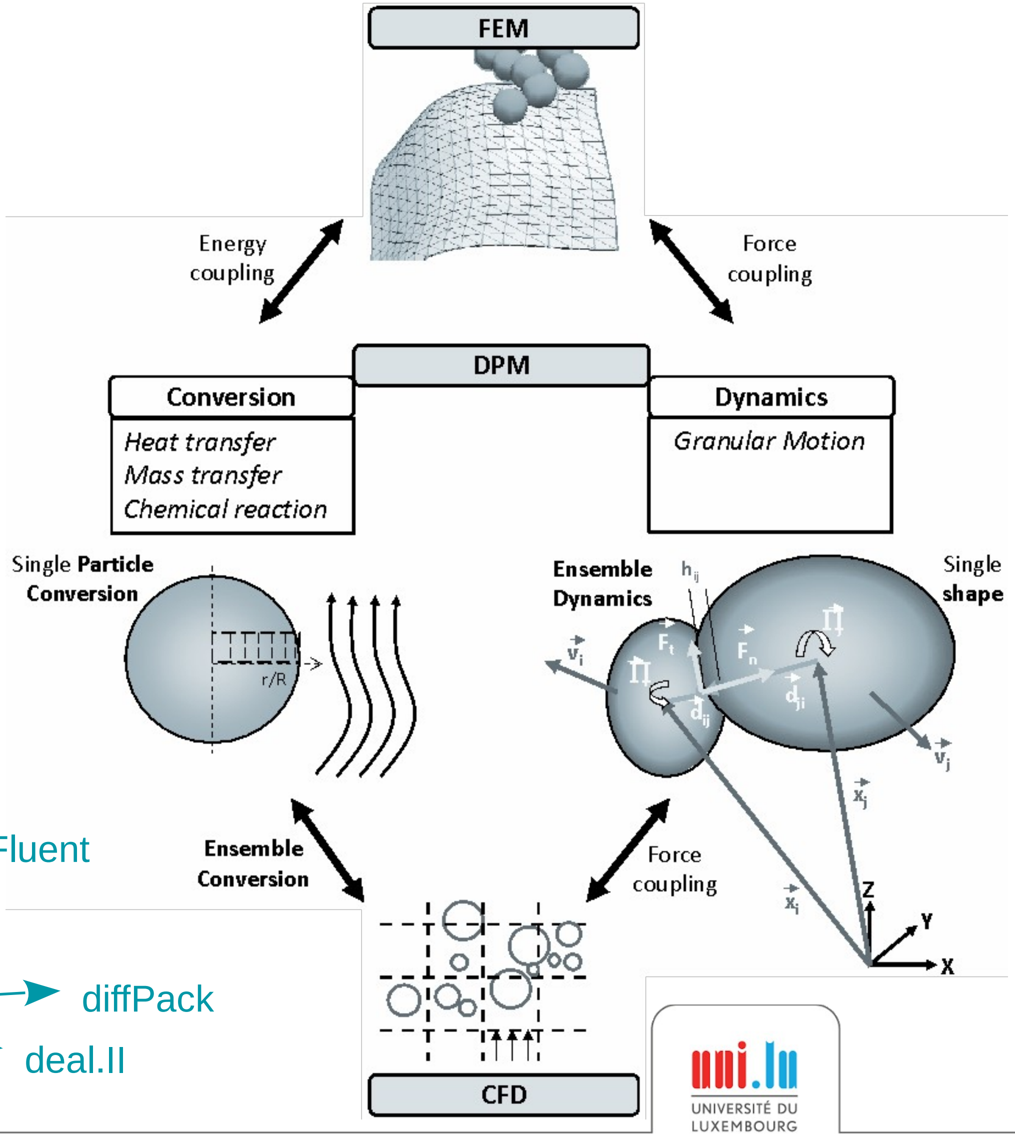
Particles Conversion

- Heat and mass transfer
- Chemical reactions

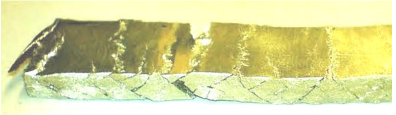
Coupled with

- Computational Fluid Dynamics (CFD) → OpenFOAM, ANSYS Fluent
- Finite Element Method (FEM) → diffPack, deal.II, CalculiX

https://luxdem.uni.lu/software/

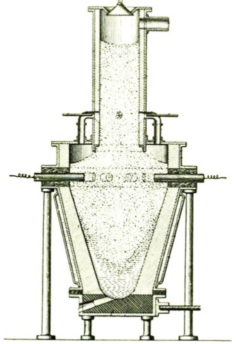


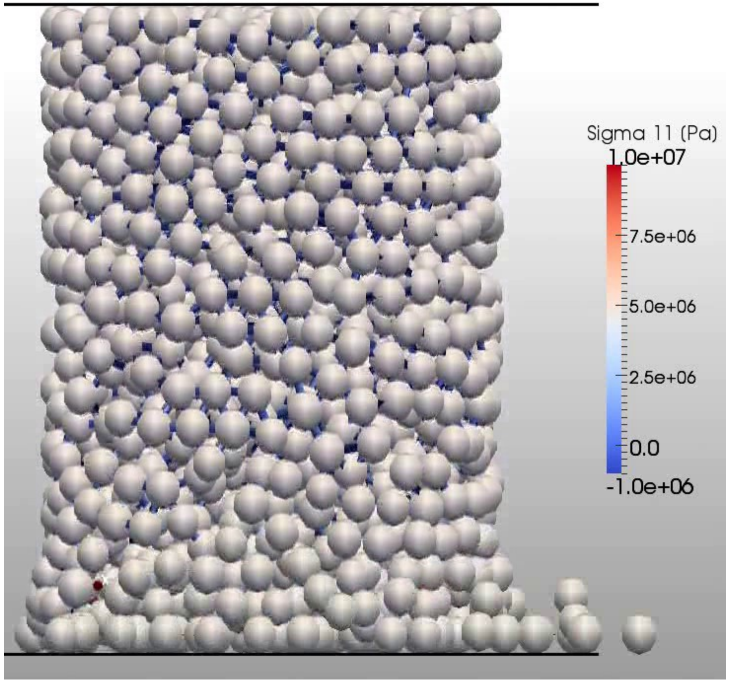
Application Examples: XDEM

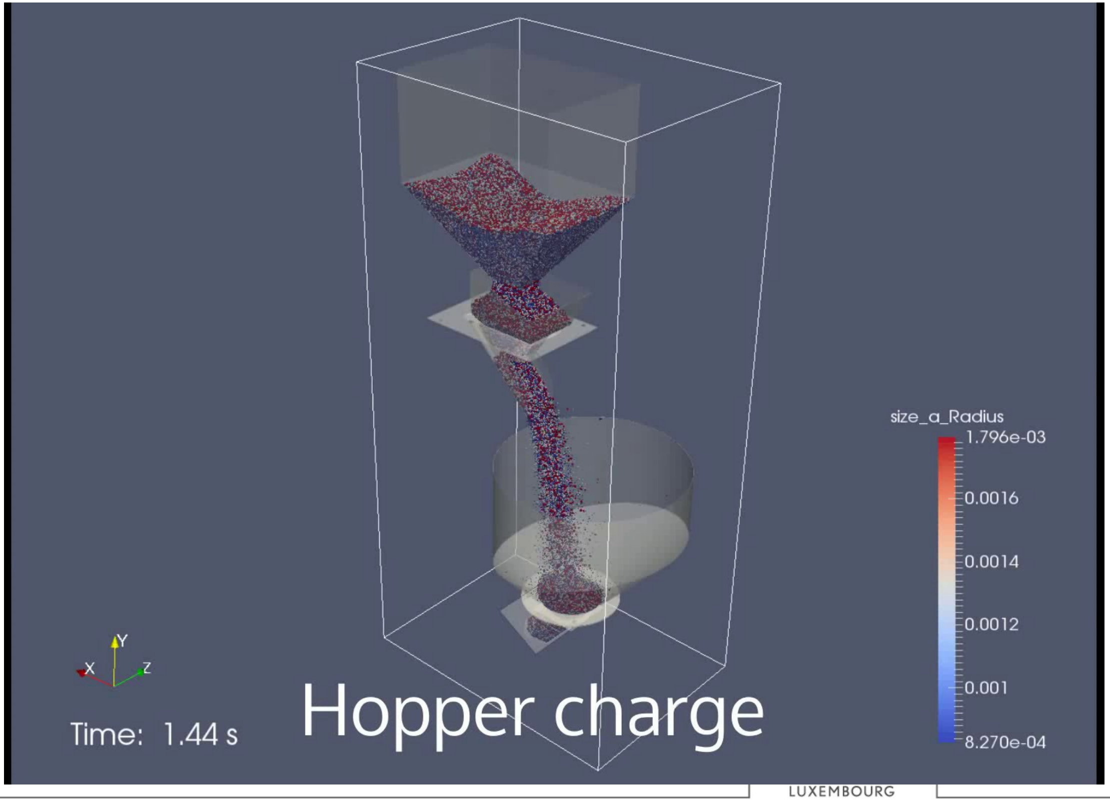


Brittle Failure

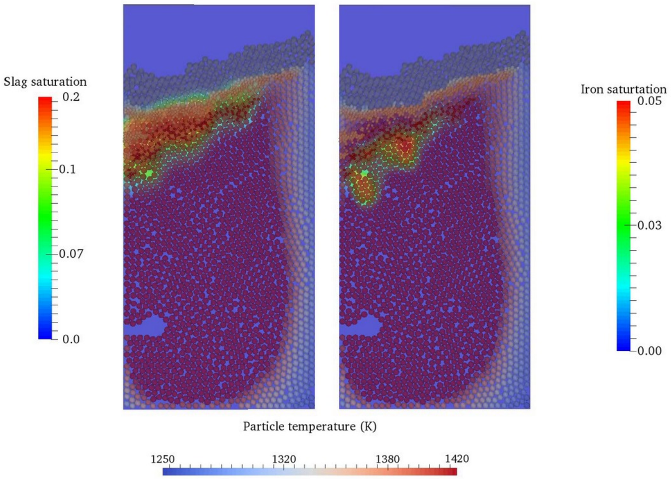
Hopper charge and discharge





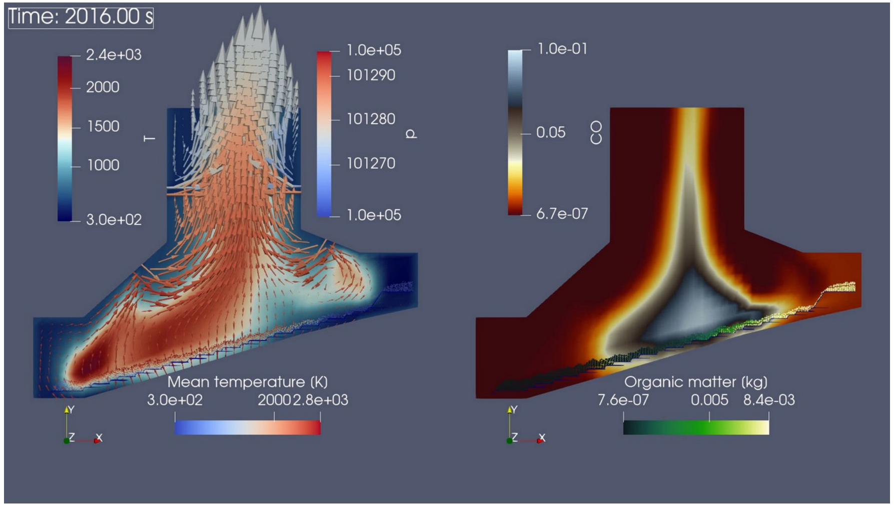


Application Examples: XDEM coupled with CFD

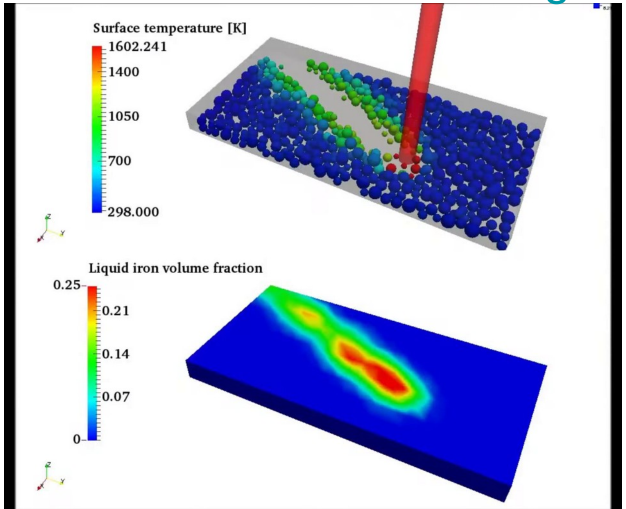


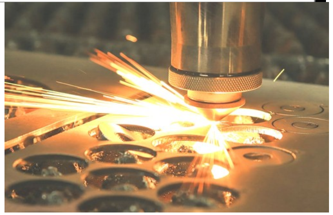
Iron & Slag production
in a Blast Furnace

Wood Conversion
in a Biomass Furnace

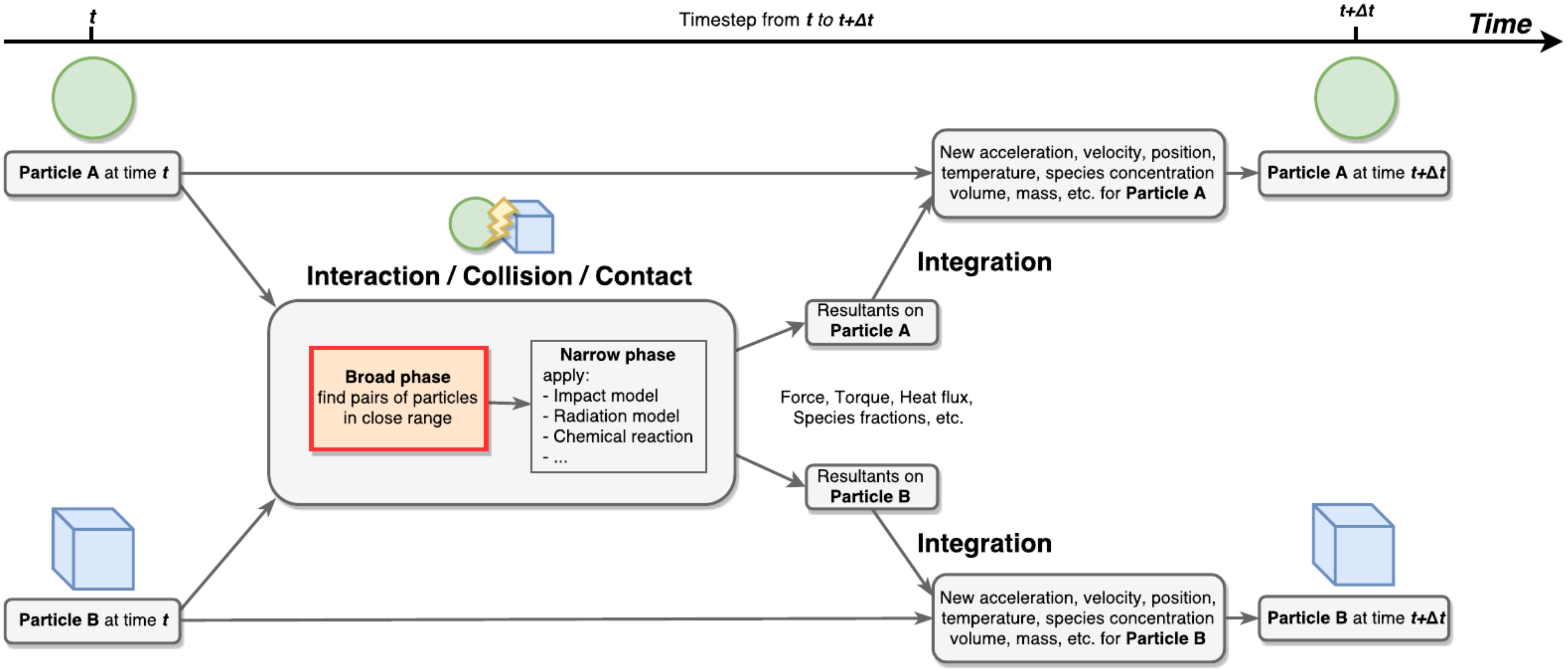


Selective Laser Melting
in Additive Manufacturing





Overview of XDEM Execution Flow



t
Timestep from t to t+Δt
t+Δt
Time
Particle A at time t
Particle B at time t
Interaction / Collision / Contact
Broad phase
find pairs of particles in close range
Narrow phase
apply:
- Impact model
- Radiation model
- Chemical reaction
- ...
Resultants on Particle A
Resultants on Particle B
Force, Torque, Heat flux, Species fractions, etc.
Integration
Integration
New acceleration, velocity, position, temperature, species concentration volume, mass, etc. for Particle A
New acceleration, velocity, position, temperature, species concentration volume, mass, etc. for Particle B
Particle A at time t+Δt
Particle B at time t+Δt

Main Computations Phases in XDEM

Interaction Detection

Broad Phase: Fast but approximate scan to identify the pairs of particles that *could* interact

- uses an approximate shape (bounding volume)

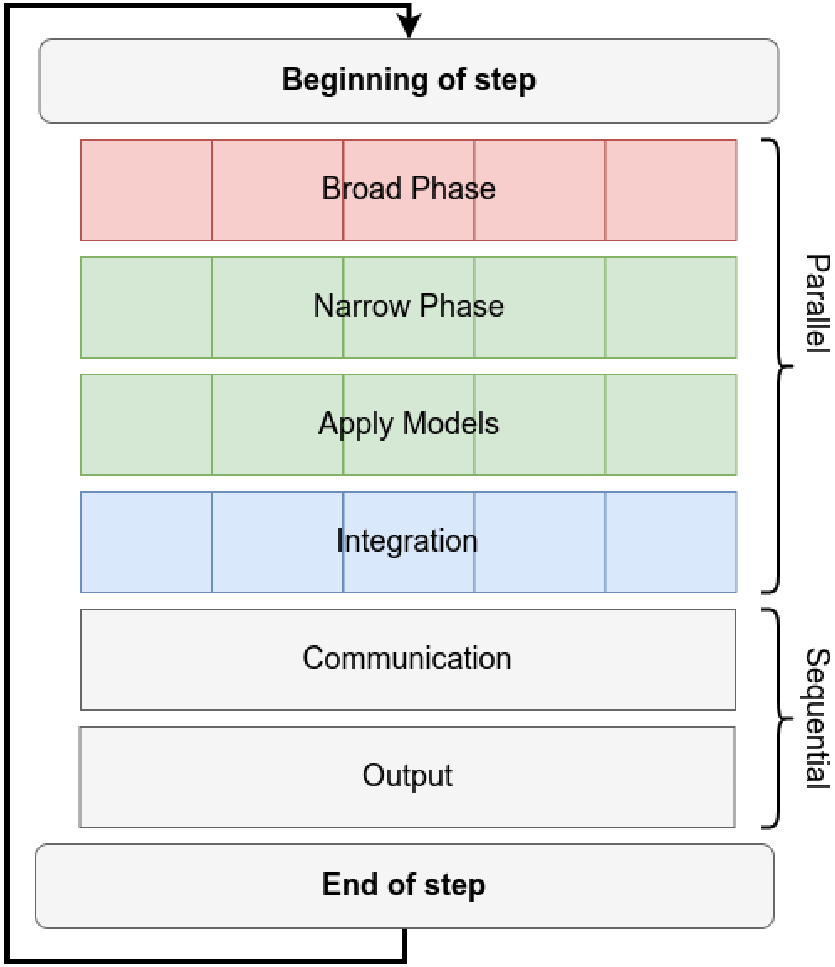
Narrow Phase: Precise collision detection on the particle pairs identified in the broad-phase

- uses the actual shape (sphere, cube, cylinder, etc.)
- calculates the distance/overlap between particles

Apply Models: Apply the physics models to each pair of interacting particles

- accumulate contributions to each particle:
  Contact → *force*, *torque*, ...
  Conduction/Radiation → *heat flux, ...*

Integration: Update the particle states by integrating the contributions from all the interacting partners



High-Performance Computing

for the Simulation of Particles

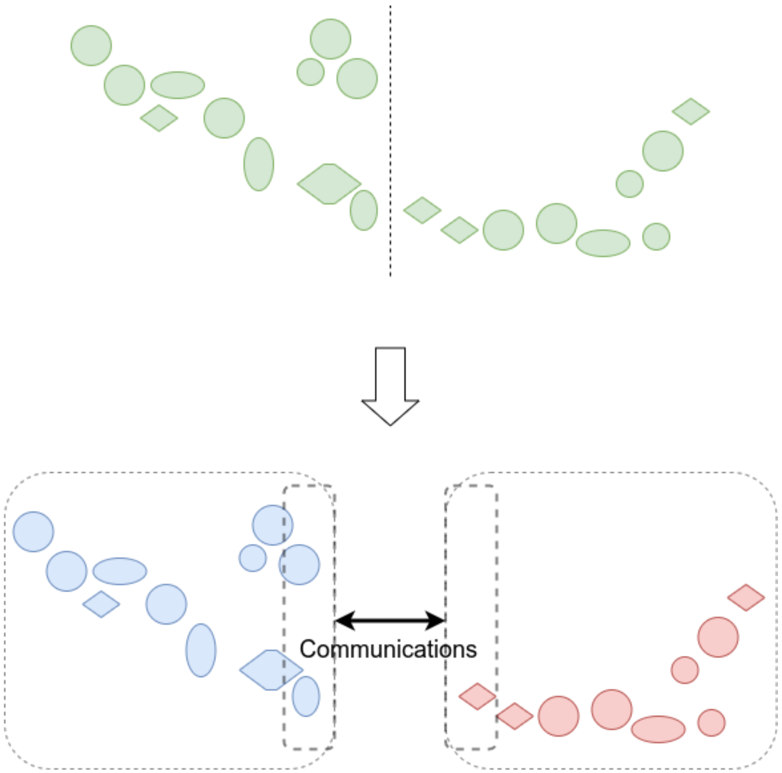
Domain Decomposition with MPI
and Load-Balancing

Domain Decomposition in XDEM

Decomposing the set of particles?

- Particles move during the simulation
- Neighborhood relations change
- Create undetected dependencies

→ Would require frequent re-partitioning



Domain Decomposition in XDEM

Decomposing the set of particles?

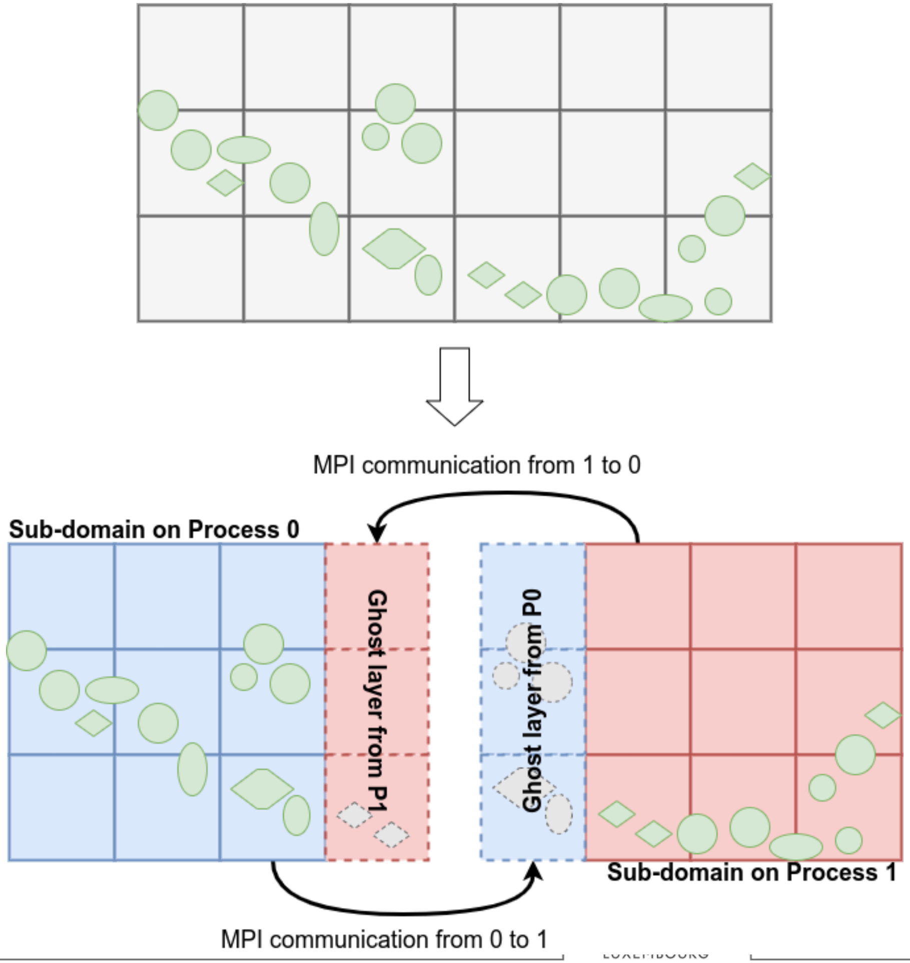
- Particles move during the simulation
- Neighborhood relations change
- Create undetected dependencies

→ Would require frequent re-partitioning

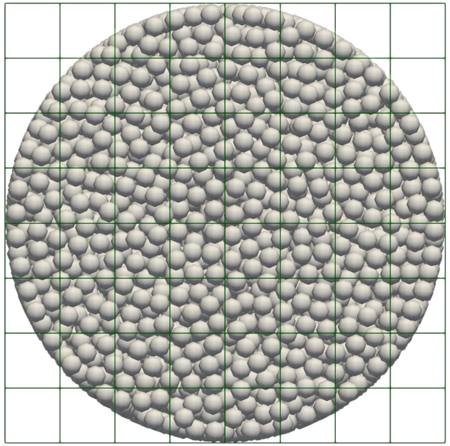
Use a static regular grid to ‘store’ particles

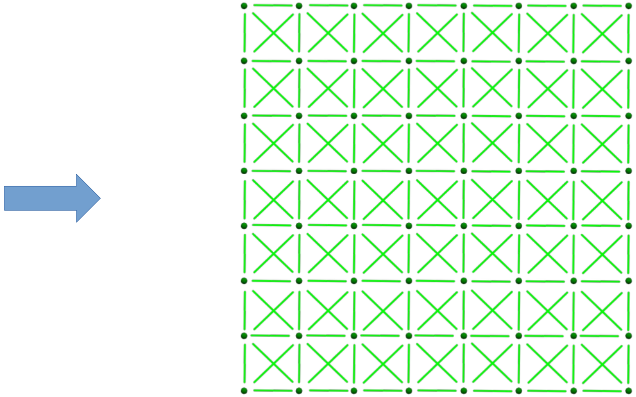
- Find location of a particle in constant time
- Size of grid cells adapted for collision detection
- No missing communication

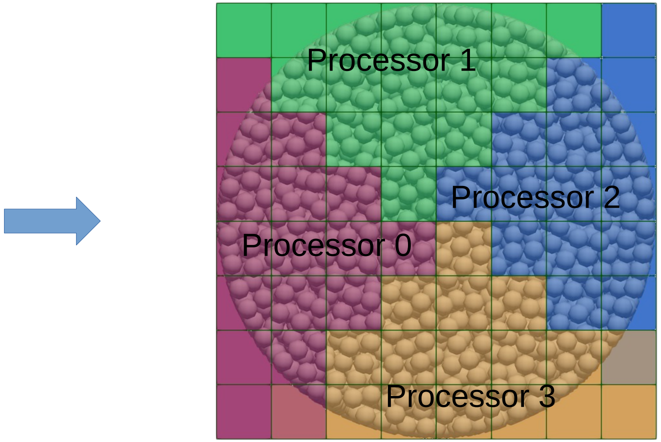
→ Re-partitioning only required in case of imbalance



Partitioning and Load-Balancing for XDEM







Particles in the cell grid

From grid to graph

- Node ← Cell
- Node weight ← *f*(nb particles)
  ~ Computation cost
- Edge ← Neighborhood relation
- Edge weight ← *g*(nb particles)
  ~ Communication cost
- Node Coordinates (topologic approaches)

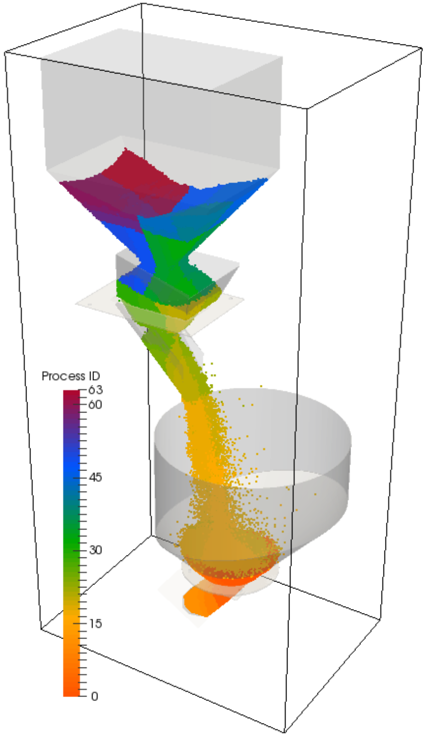
Partitioning algorithm

- Orthogonal Recursive Bisection
- METIS
- SCOTCH
- Zoltan PHG, RCB, RIB, ...
- etc.

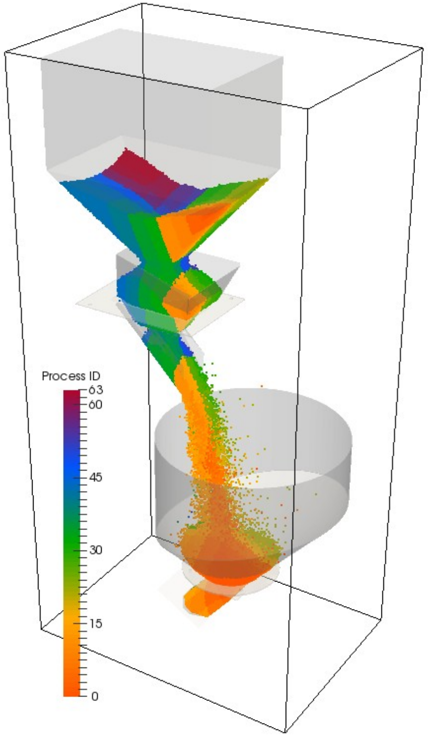
Objectives

- Balance the computation cost
- Minimize the communication cuts

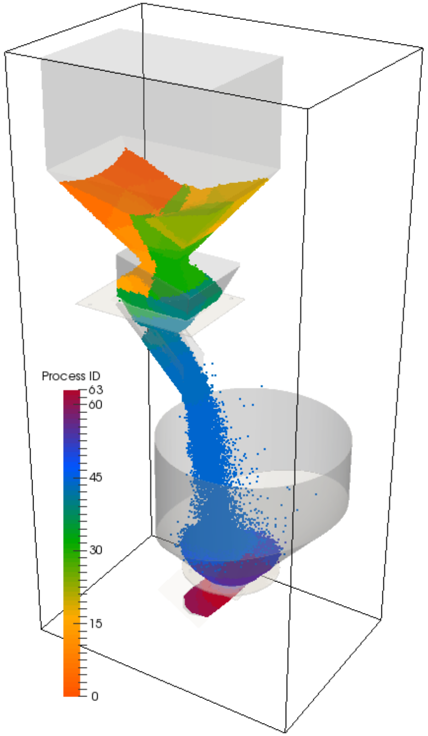
Example of Load-Balancing



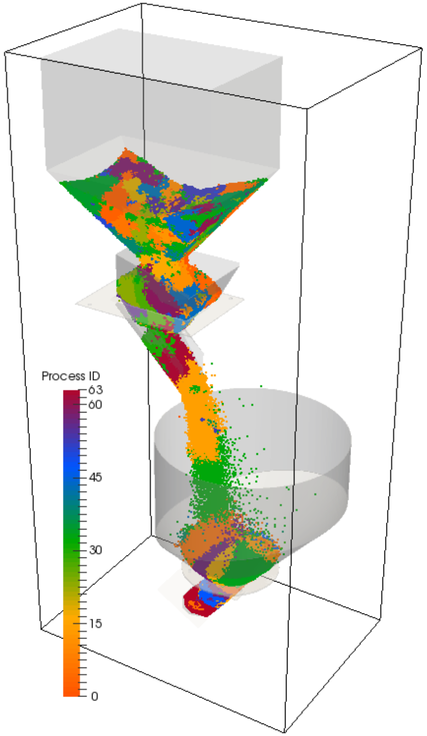
Zoltan RCB
(Recursive Coordinate Bisection)



ORB
(Orthogonal Recursive Bisection)



Zoltan RIB
(Recursive Inertial Bisection)



SCOTCH K-way

Weight estimation for load-balancing

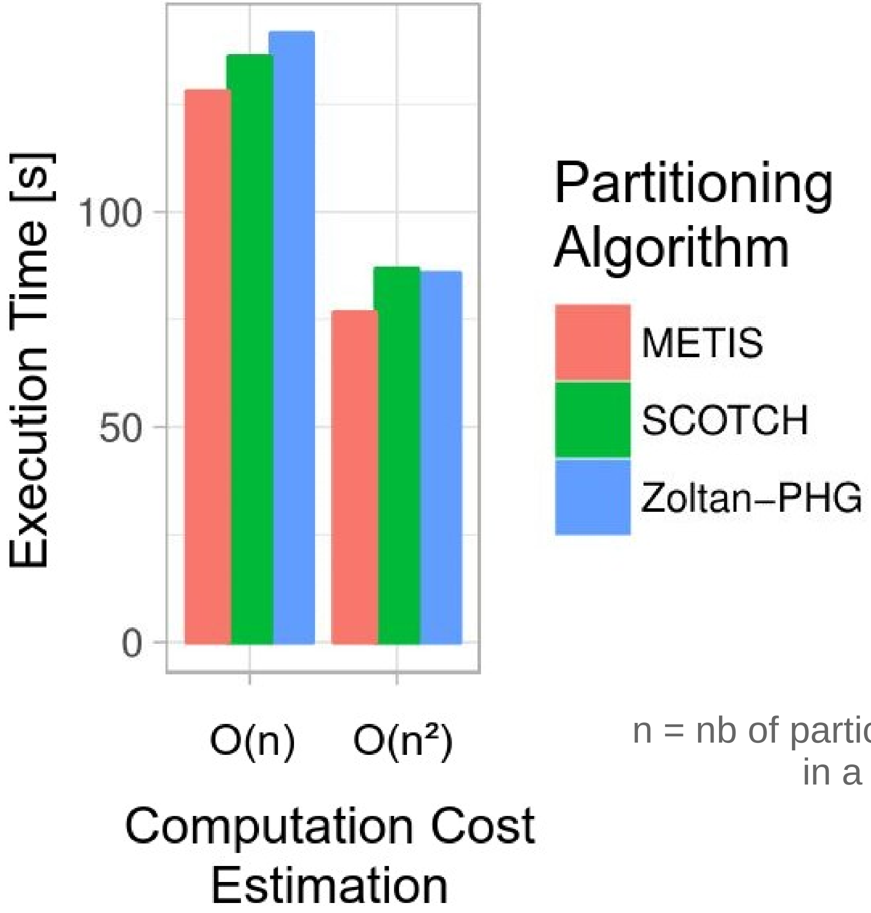
How to estimate the computing cost ?

- Difficult to measure at the level of a single cell
- Multiple phases and different complexities

Computation Phase	*Complexity*
Broad-phase	O((nb particles)^2)
Narrow-phase	O(nb interactions)
Apply Models	O(nb interactions)
Integration	O(nb particles)

- Nb of interactions is difficult to estimate

→ **Work in progress**



n = nb of particles in a cell

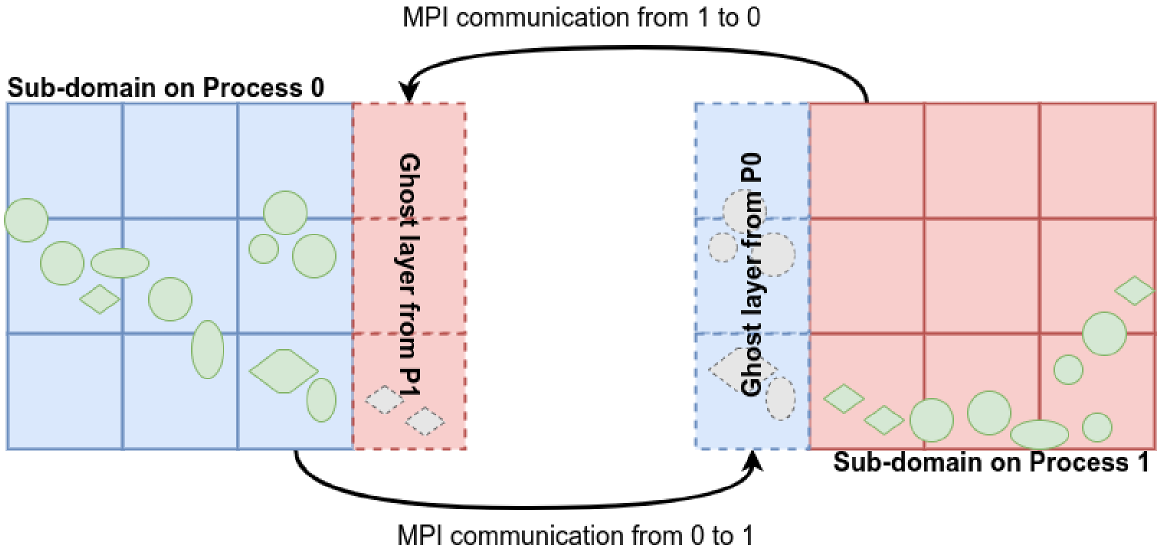
High-Performance Computing

for the Simulation of Particles

Fine grain parallelization with OpenMP

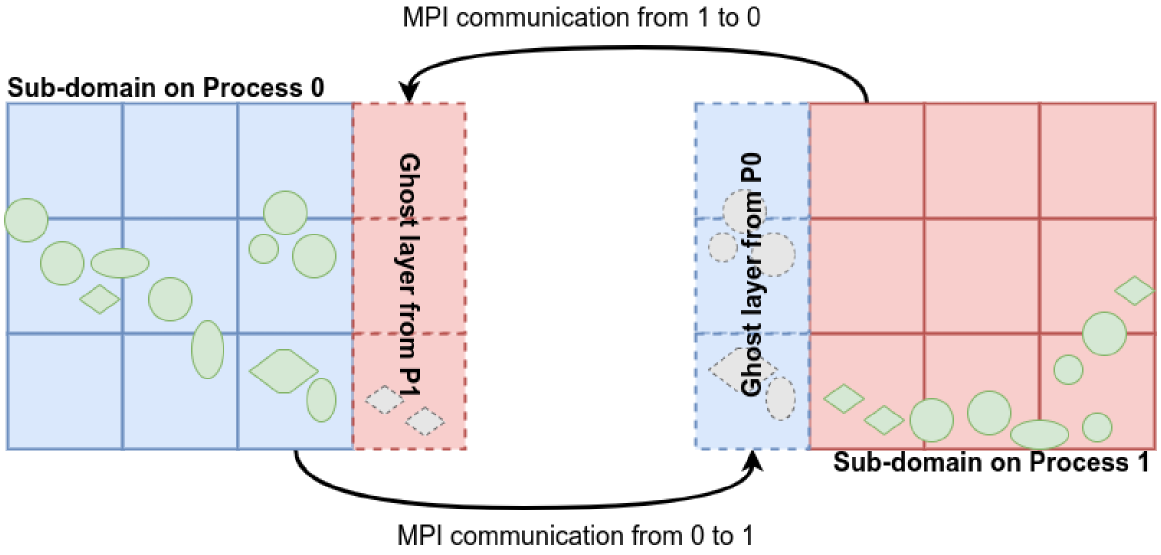
Hybrid Parallelization MPI+OpenMP of XDEM

Decomposed Particle Domain

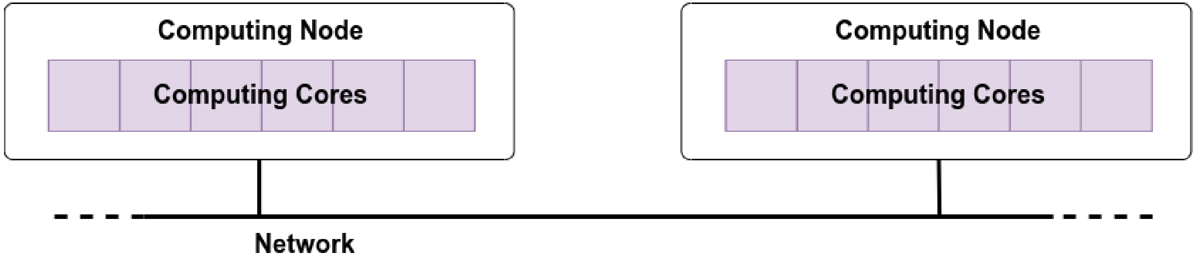


Hybrid Parallelization MPI+OpenMP of XDEM

Decomposed Particle Domain

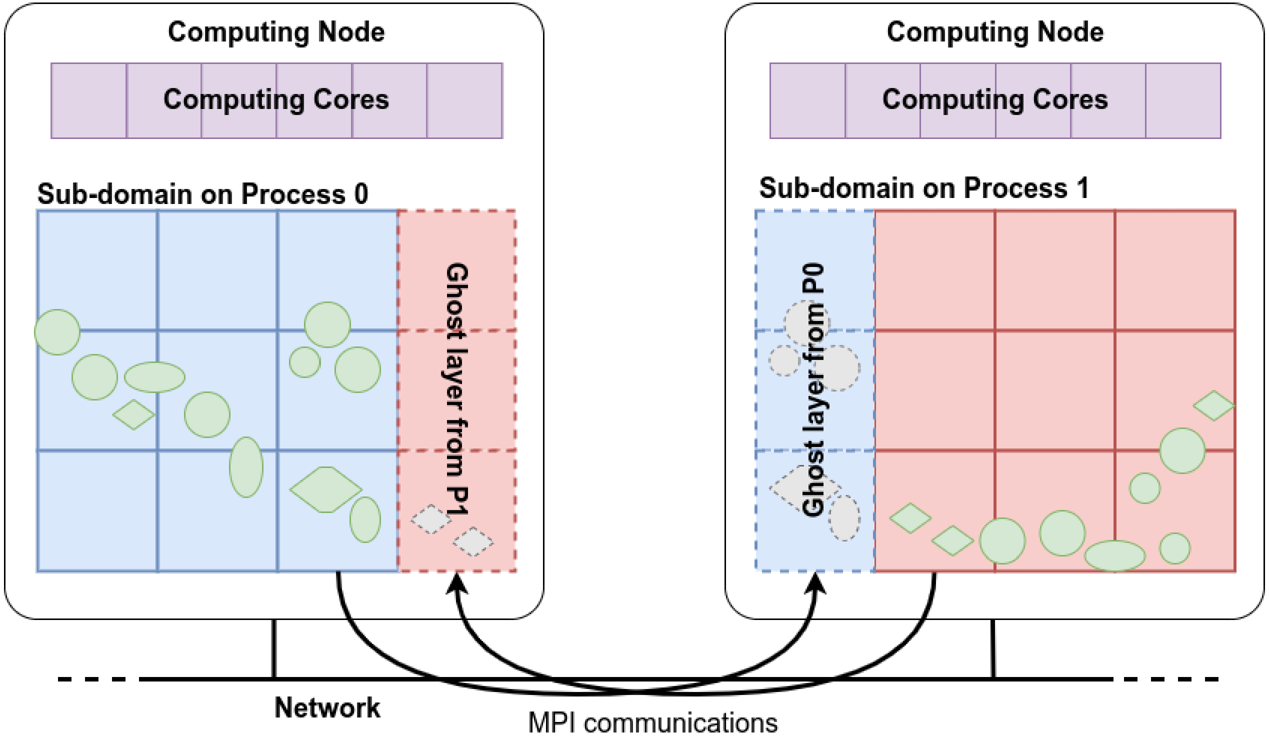


Computing Platform



Hybrid Parallelization MPI+OpenMP of XDEM

Sub-domains distributed on computing nodes with MPI
→ Coarse grain //



Hybrid Parallelization MPI+OpenMP of XDEM

Sub-domains distributed on computing nodes with MPI
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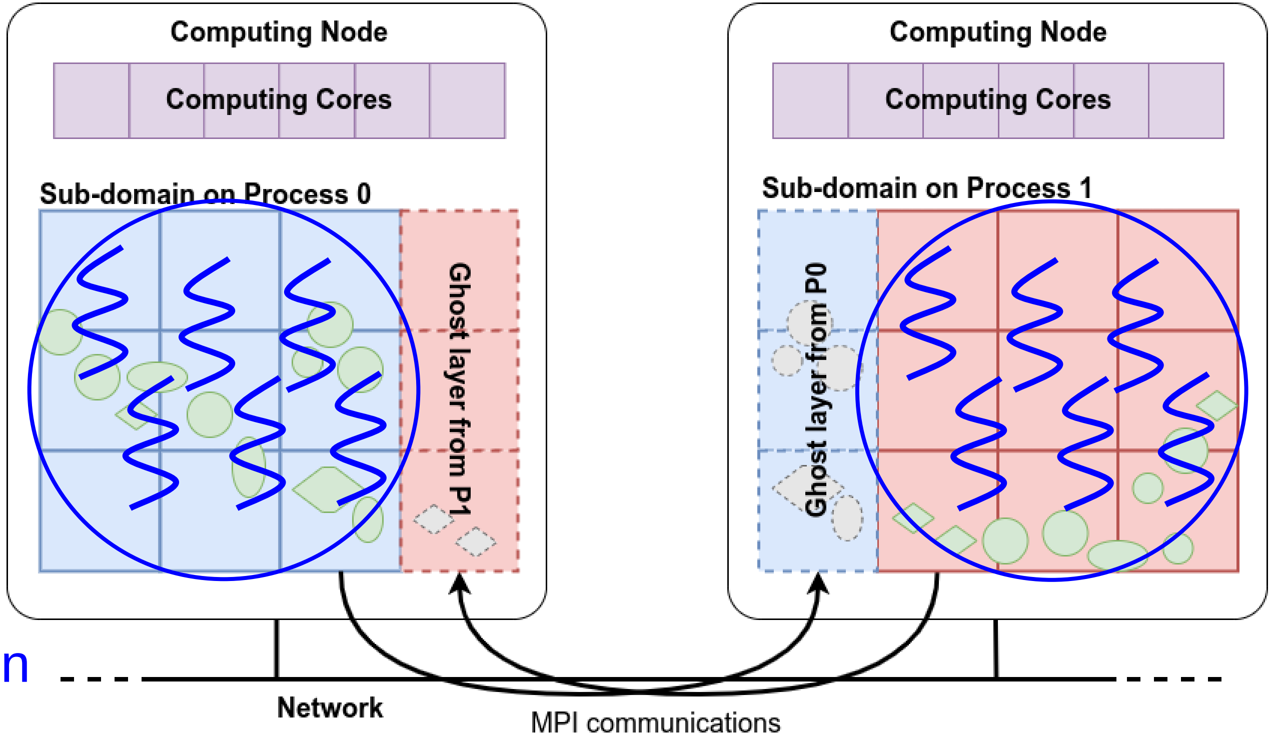


Intra-subdomain parallelization with OpenMP
→ Fine grain //

XDEM parallelization with OpenMP

Parallelization at a fine grain:

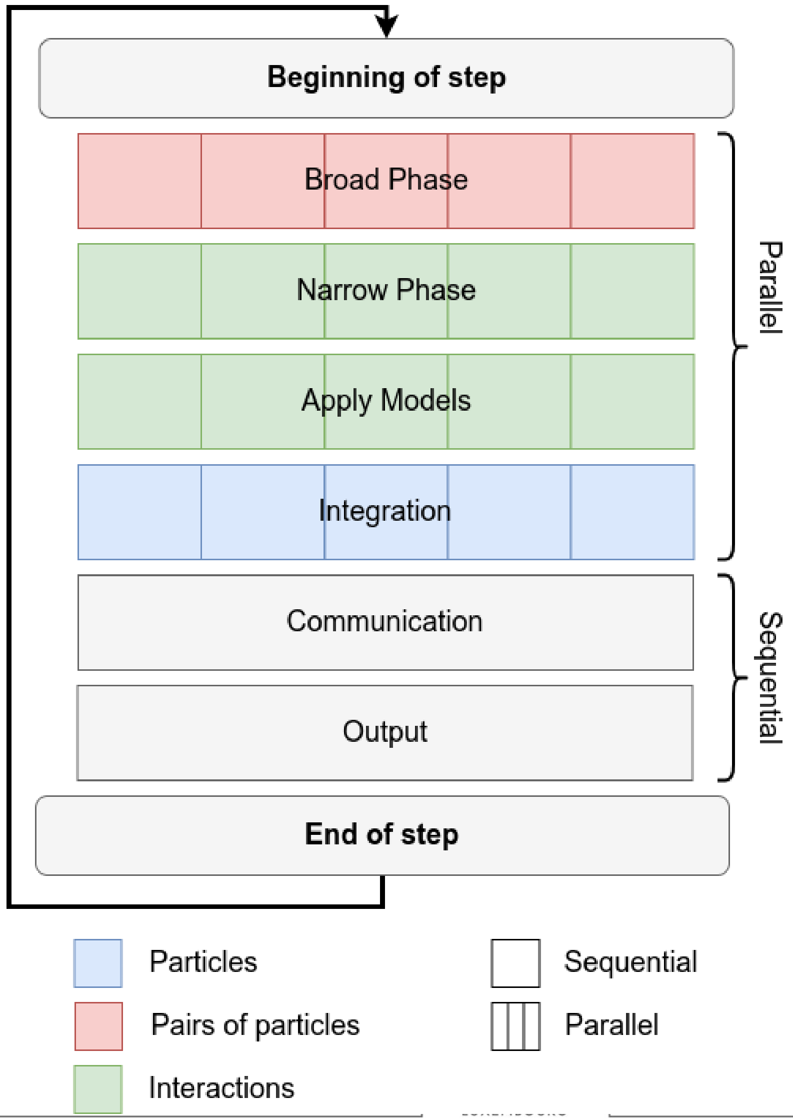
- Particles, Pairs of particles and Interactions

Guided by the type of accesses:

- Iterate on the objects being modified to avoid concurrent accesses (when possible)
- Use containers with random access iterators

	Read Access	Write Access	Iteration on
Broad Phase	Particles	Interactions	Particle pairs
Narrow Phase	Interactions	Interactions	Interactions
Apply Models	Interactions	Particles	Interactions
Integration	Particles	Particles	Particles

Potential concurrent accesses!



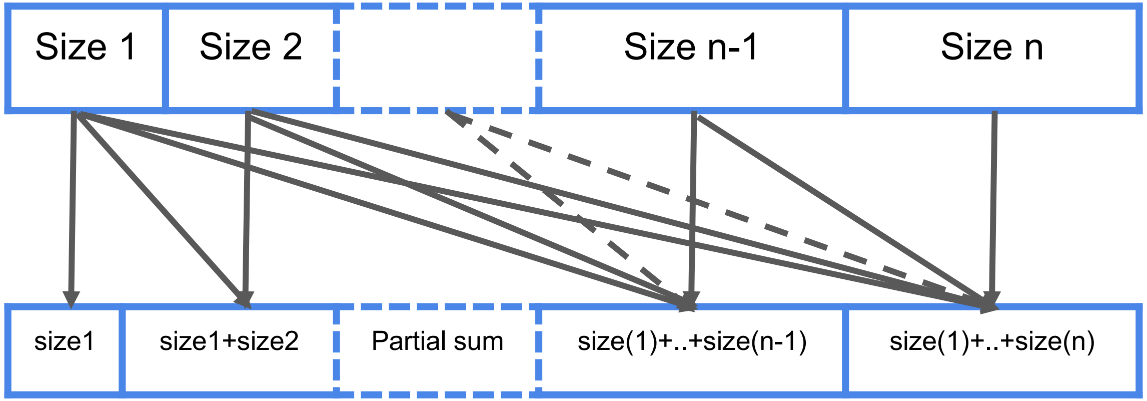
Concurrency write

How to fill Interactions vector concurrently?

→ Unkown number of interactions

Solution

- Each thread fills a private **`deque`**
- Perform a partial sum of sizes
- Copy in shared vector at the position defined by the partial sum
- Synchronization barrier at the end



→ No critical or atomic regions

Memory allocator

XDEM C++ code is highly dynamic

➔ Intensive calls to the memory allocator

Default **glibc** memory allocator

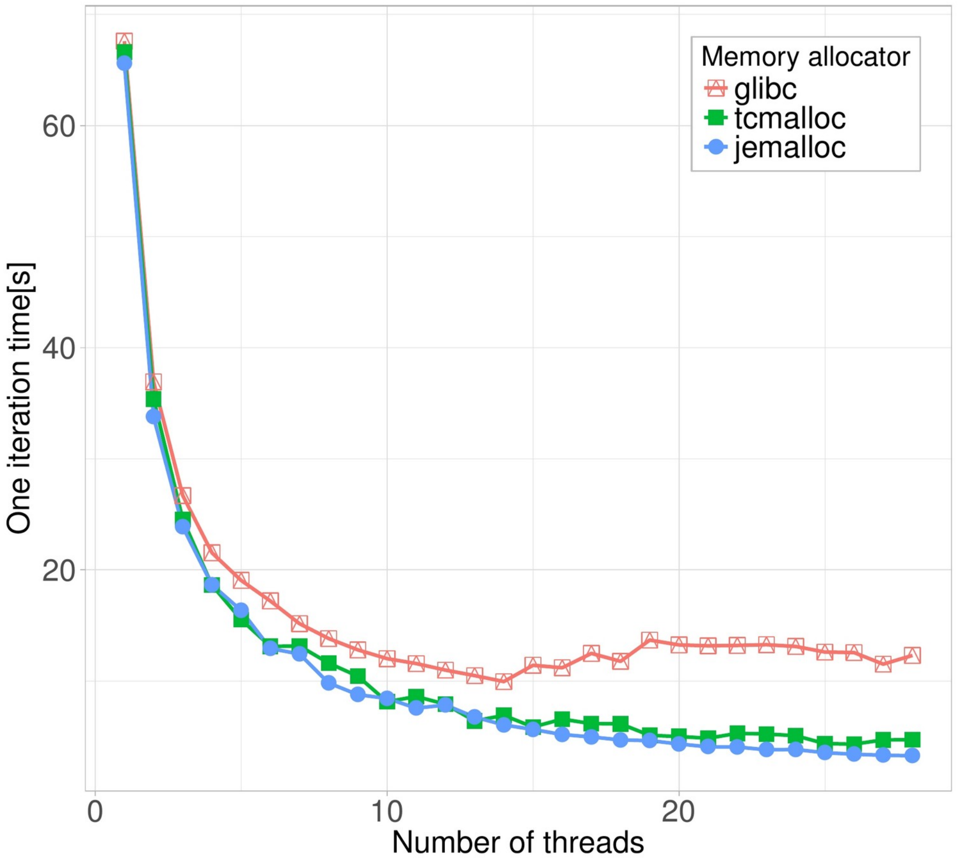
- uses locks internally

➔ Limits the scalability of threaded executions

Optimized memory allocators

- **Jemalloc** based on independent arenas
- **TCMalloc** based thread cache

→ **3-4 times faster on 28 cores**

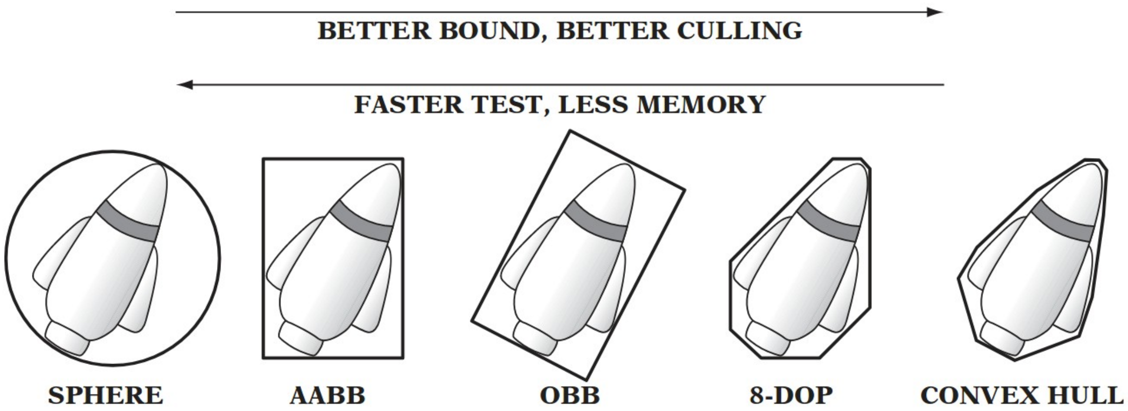


High-Performance Computing

for the Simulation of Particles

Faster Broad-Phase with Roofline Analysis

Bounding Volumes in XDEM Broad-phase

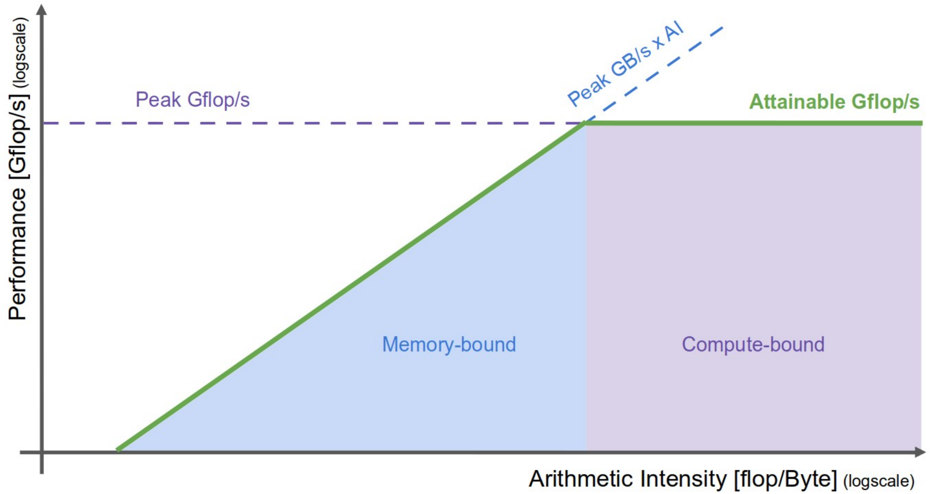


Real-Time Collision Detection, by Christer Ericson, 2005.

Which bounding volume for the broad-phase?

- Bounding Sphere (BS)?
- Axis Aligned Bounding Box (AABB)?

Roofline Analysis for Bounding Volumes



- Broad-phase is memory-bounded

Intersection of 2 bounding volume?

	Memory	**Complexity of ∩**	**AI**
Bounding Sphere	2 x 4 reals (position + radius)	11 arithmetic ops 1 comparison	**1.38 flop/real**
Axis Aligned Bounding Box	2 x 6 reals (upper + lower corners)	6 comparisons 5 logical AND	0.5 flop/real

- Bounding Spheres release the pressure on memory bandwidth
- Using `float` type instead `double` also reduces memory accesses

⇒ Use Bounding Spheres of `floats`

High-Performance Computing

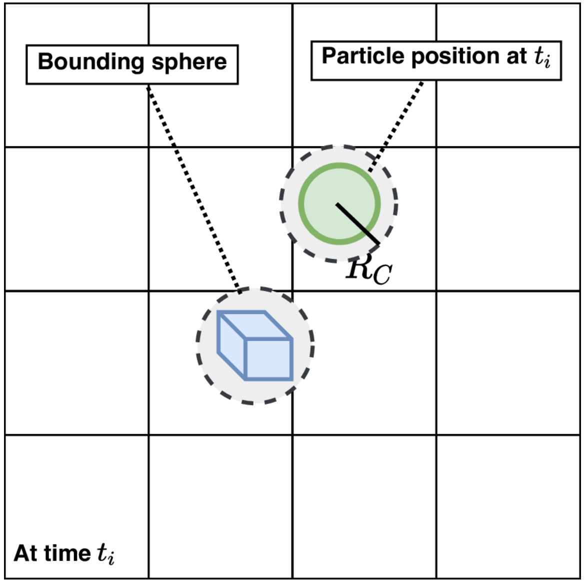
for the Simulation of Particles

Verlet Buffer approach for Collision Detection

Verlet Buffer for Collision Detection in XDEM 1/3

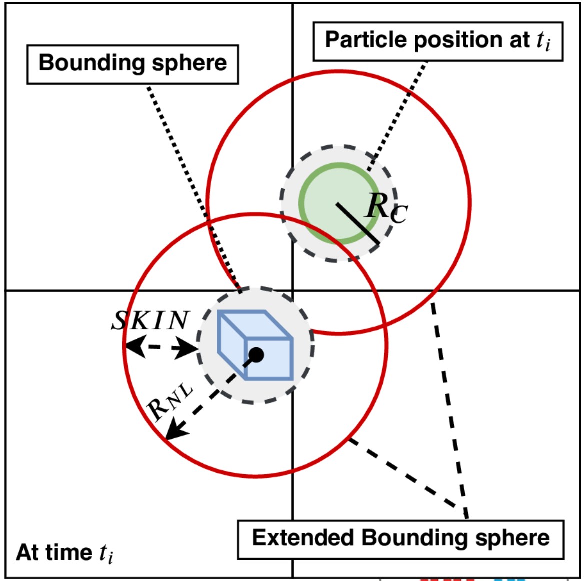
Idea → Inspired from Computer “Experiments” on Classical Fluids. I. Thermodynamical Properties of Lennard-Jones Modecules by L. Verlet, 1967.

- Extend the range of collision detection in the Broad Phase
- Potential collision partners are valid for many iterations



Extend Bounding Spheres with

Skin = **K** . $V_{particle}$. dt

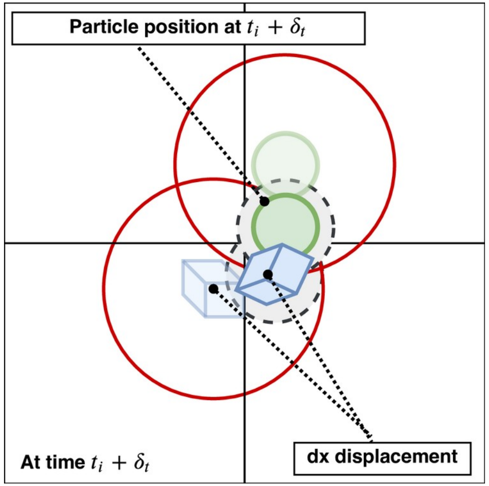


Verlet Buffer for Collision Detection in XDEM 2/3

Next Timesteps

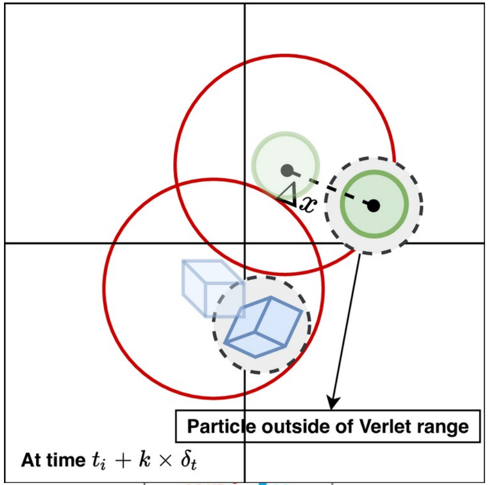
If all particles are still within their extended bounding spheres

- ➔ Skip the Broad Phase
- ➔ Proceed with the Narrow Phase using previously-calculated list of interaction pairs



If one particle exits its bounding spheres

- ➔ Re-calculate the Broad Phase with new extended bounding spheres

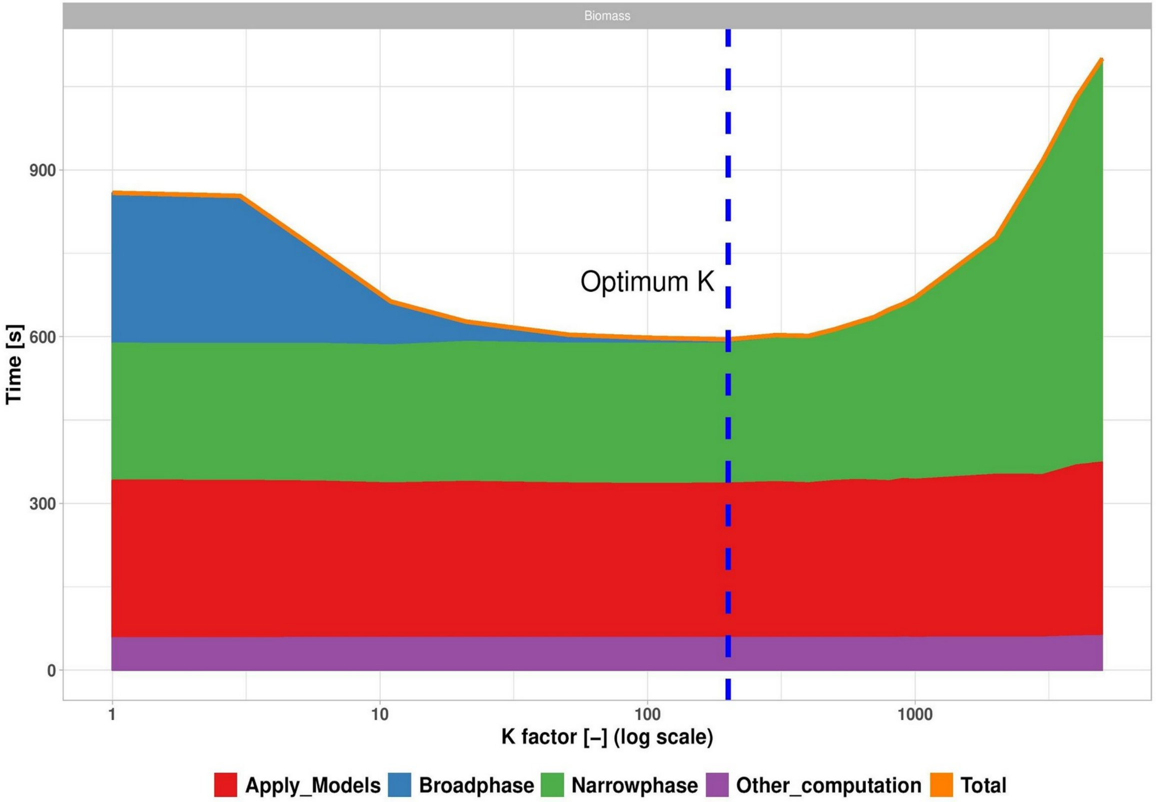

Δx
Particle outside of Verlet range
At time $t_i + k \times \delta_t$

- Narrow Phase is always executed
- Identical results are guaranteed

Verlet Buffer for Collision Detection in XDEM 3/3

Increasing **K**

- Increasing cost of **Narrow Phase**
- Increasing cost of each **Broad Phase**
- But less executions of **Broad Phase**
- Less time spent in **Broad Phase** overall



K = 200 is a good default value

- Simulation time reduced by 18% to 81%

Regression model for K trained on examples

- Best **K** value between 150 and 600
- Additional improvement between 0% to 26%

Going further:

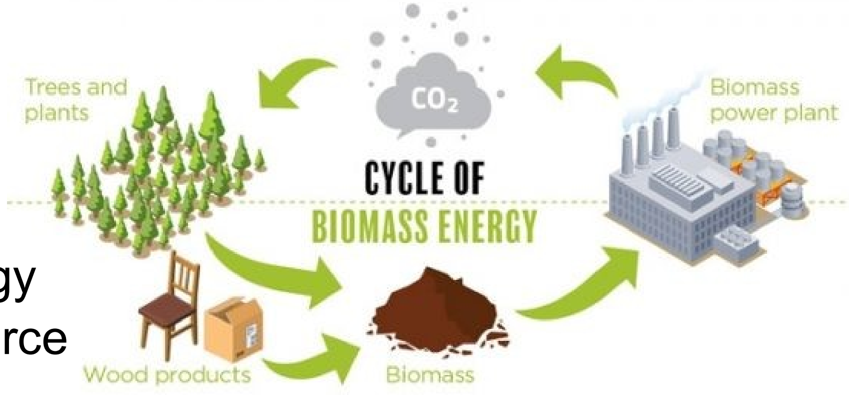
Discrete Element Method (DEM)

+

Computational Fluid Dynamics (CFD)

Parallel Multi-Physics Simulation
of a Biomass Furnace

Biomass Combustion



Biomass combustion (e.g. wood chips)

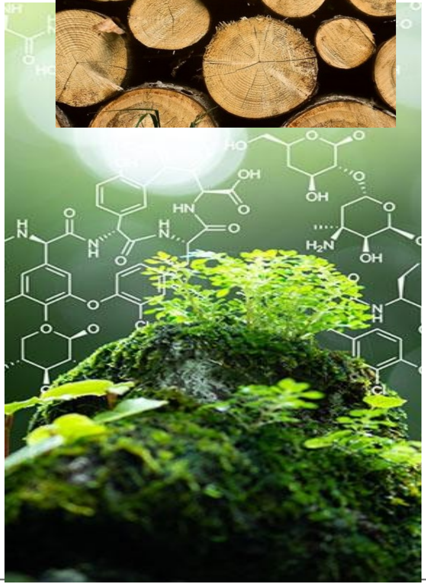
- widely used for generating electric and thermal energy
- renewable and potentially carbon-neutral energy source

Combustion process

- very complex
- requires advanced techniques to minimize harmful gas emissions

Alternative biomass

- wood waste, straw, bark, olive pits, nut shells, grain husks, bagasse, etc.
- can cause problems due to their chemical composition, ash melting temperature, humidity, ash content, calorific value and others.



Combustion process in a biomass furnace

Combustion chamber of a biomass furnace

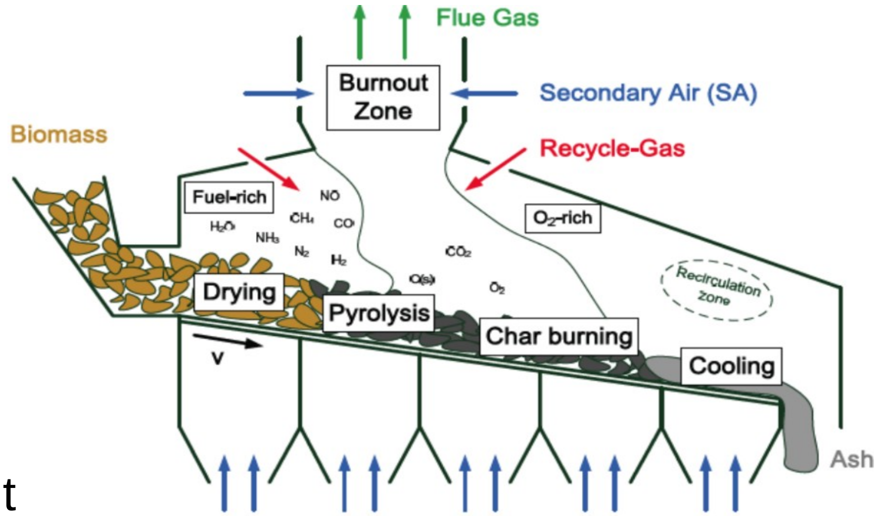
- forward acting grate
- transports the fuel through the furnace

The fuel undergoes a number of steps

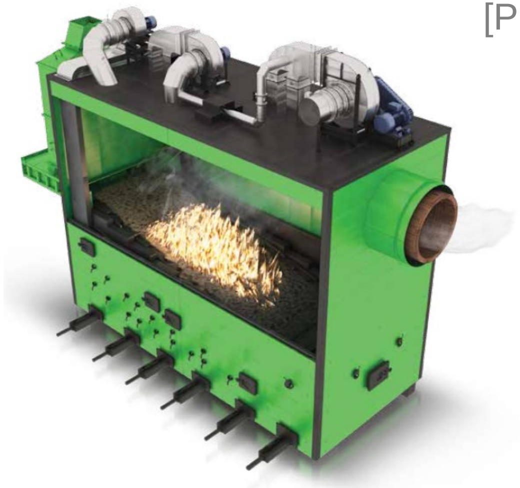
- drying, pyrolysis, char burning, cooling in which it releases hydrocarbons
- hydrocarbons are burned in the gas phase

Use **numerical simulations**

- to study efficiency and performance
- and reduce the costs of experiments



[Paces and Kozek, 2011]



Numerical Approach for Biomass Furnace: **Multi-Physics Simulation**

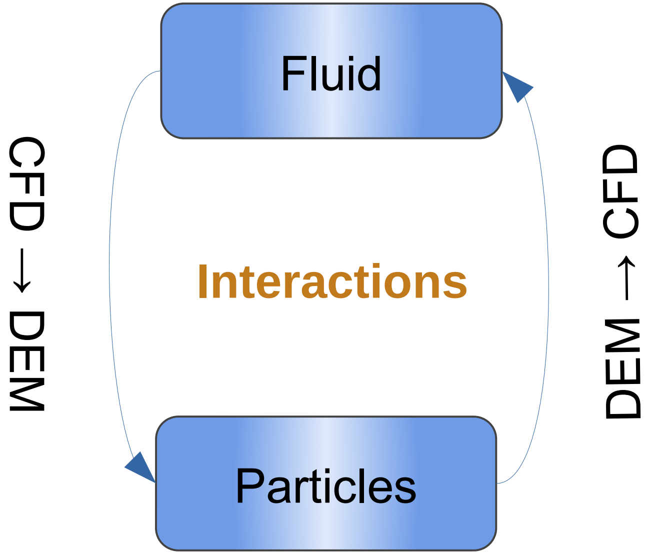
Two-way **volume coupling** between
Discrete Element Method (DEM) and
Computational Fluid Dynamics (CFD)

XDEM (Lagrangian) for:

- Motion and collisions of biomass particles
- Thermodynamic Conversion of biomass particles

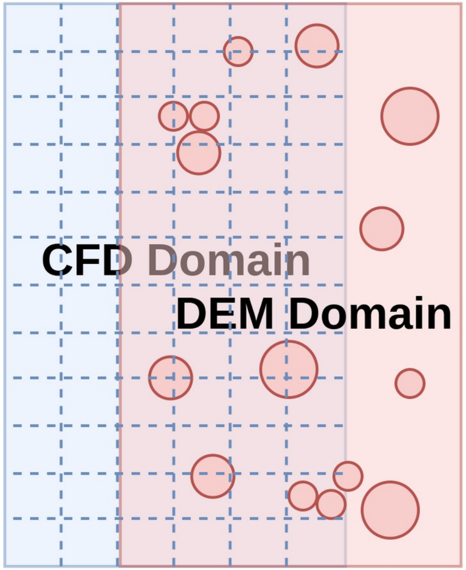
OpenFOAM (Eulerian) for:

- Flow of gas phase
- Reactions in the gas phase



CFD-DEM coupling is required to capture the physics of biomass furnaces and offers unprecedented insight.

CFD-DEM Parallel Coupling: Challenges

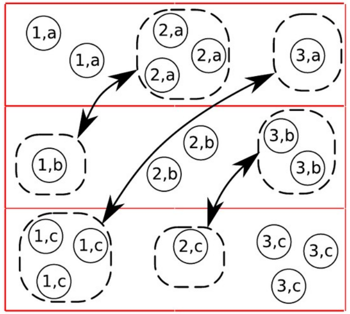


Challenges in CFD-XDEM parallel coupling

- Combine different independent software
- **Volume coupling** ⇒ Large amount of data to exchange
- Different distributions of the computation and of the data
- DEM data distribution is dynamic
- Data interpolation between meshes

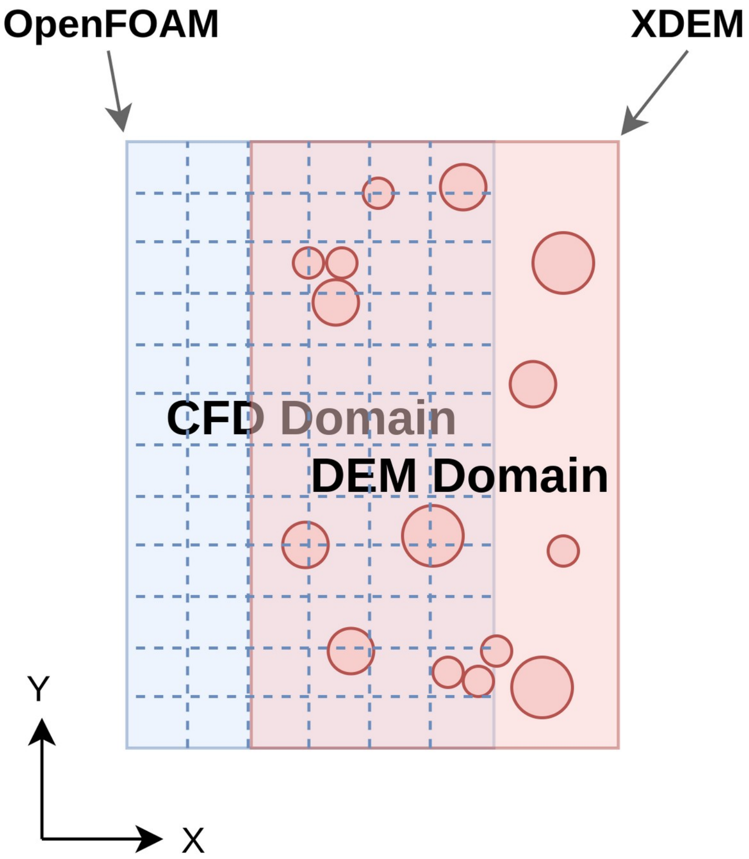
Classical Approaches

- Each software partitions its domain independently
- Data exchange in a peer-to-peer model



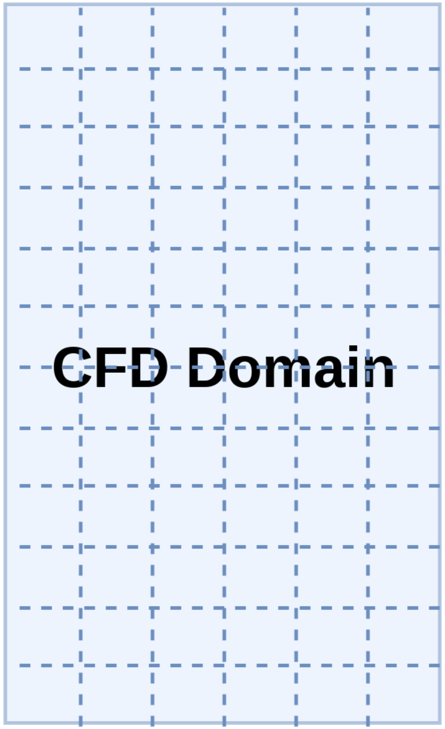
SediFoam [Sun2016]

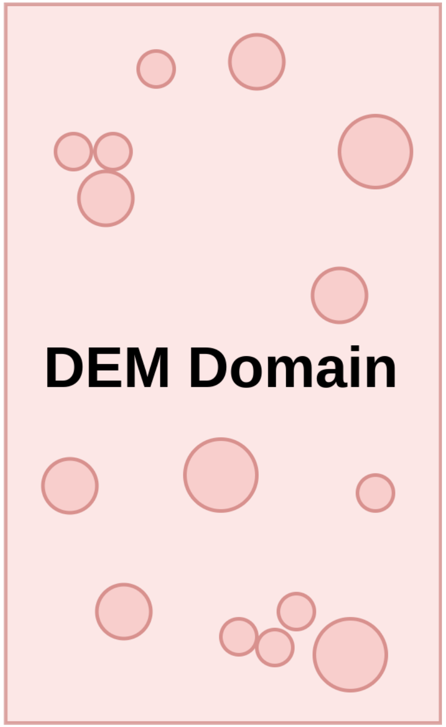
CFD-DEM Parallel Coupling: Challenges



The domains overlap in space

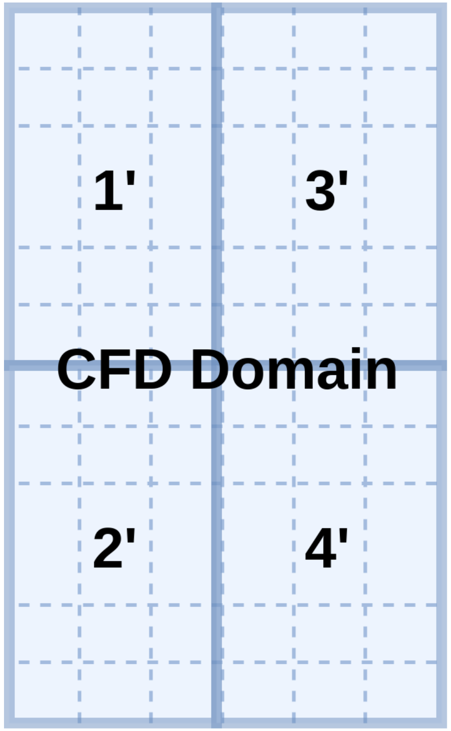
CFD-DEM Parallel Coupling: Challenges

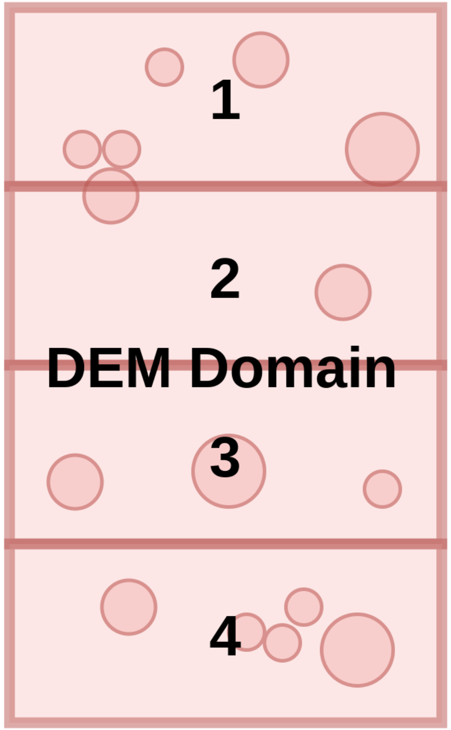




CFD-DEM Parallel Coupling: Challenges

Classical Approach: the domains are partitioned independently





CFD-DEM Parallel Coupling: Challenges

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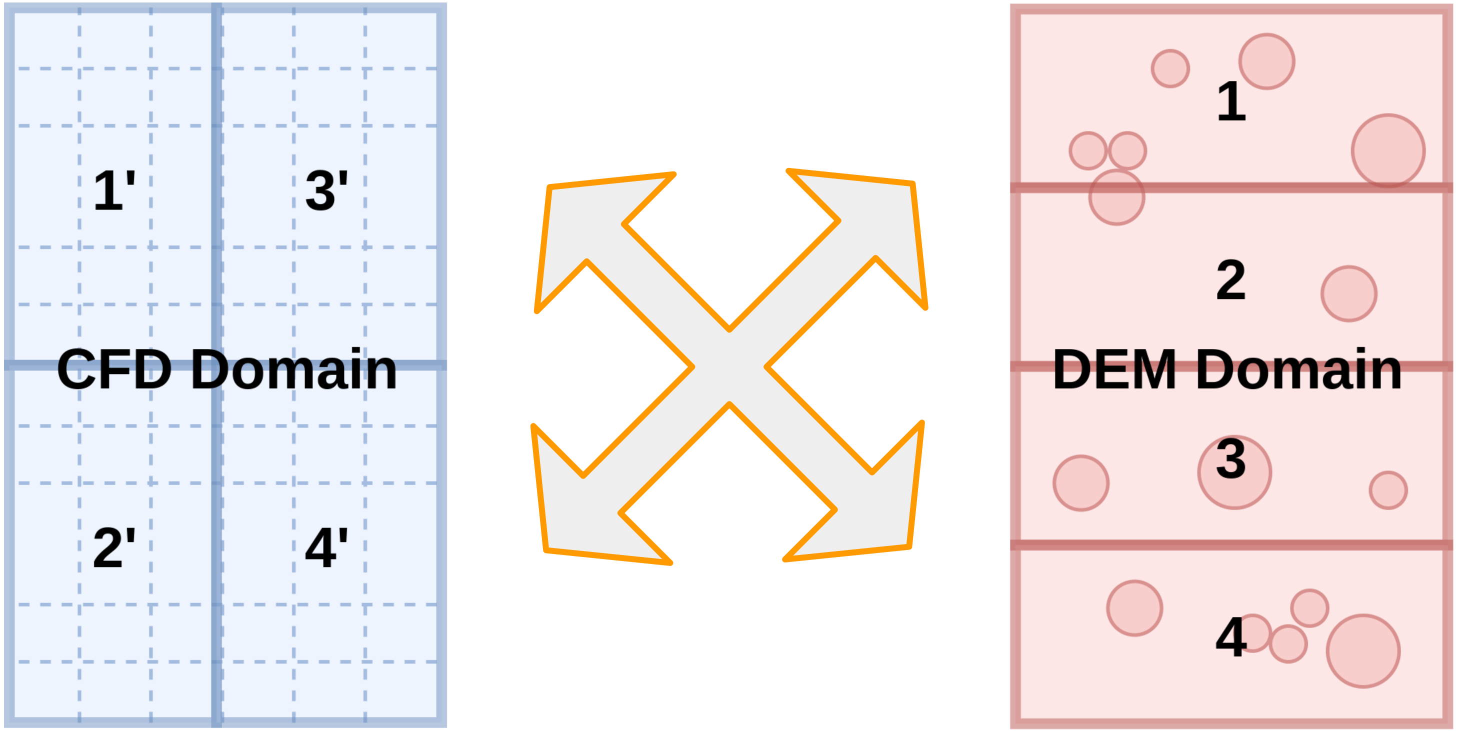
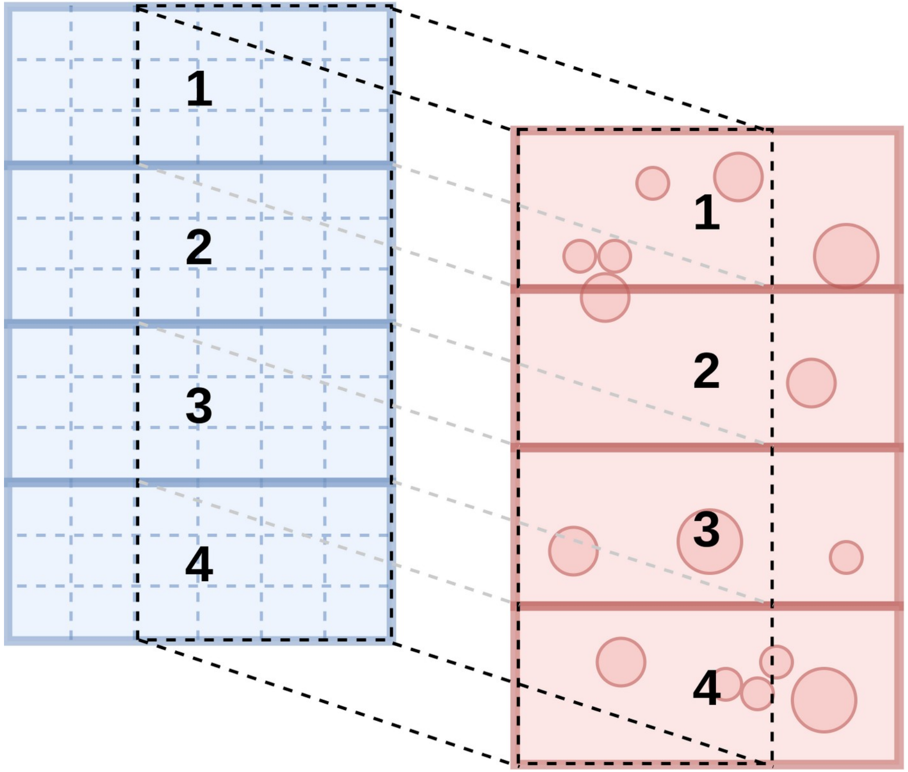


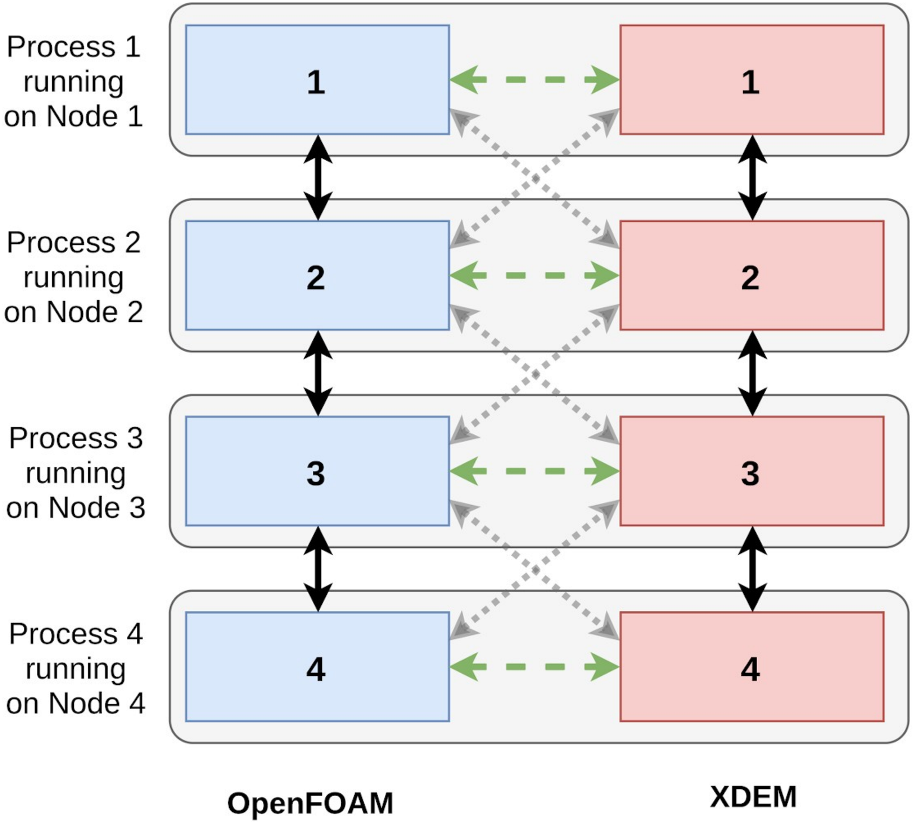
Complex pattern and large volume of communication

Co-located Partitioning Strategy



Domain elements co-located in domain space are assigned to the same partition

Co-located Partitioning Strategy: communication


Process 1 running on Node 1
Process 2 running on Node 2
Process 3 running on Node 3
Process 4 running on Node 4
1
2
3
4
1
2
3
4
OpenFOAM
XDEM

Intra-physics Data Exchange

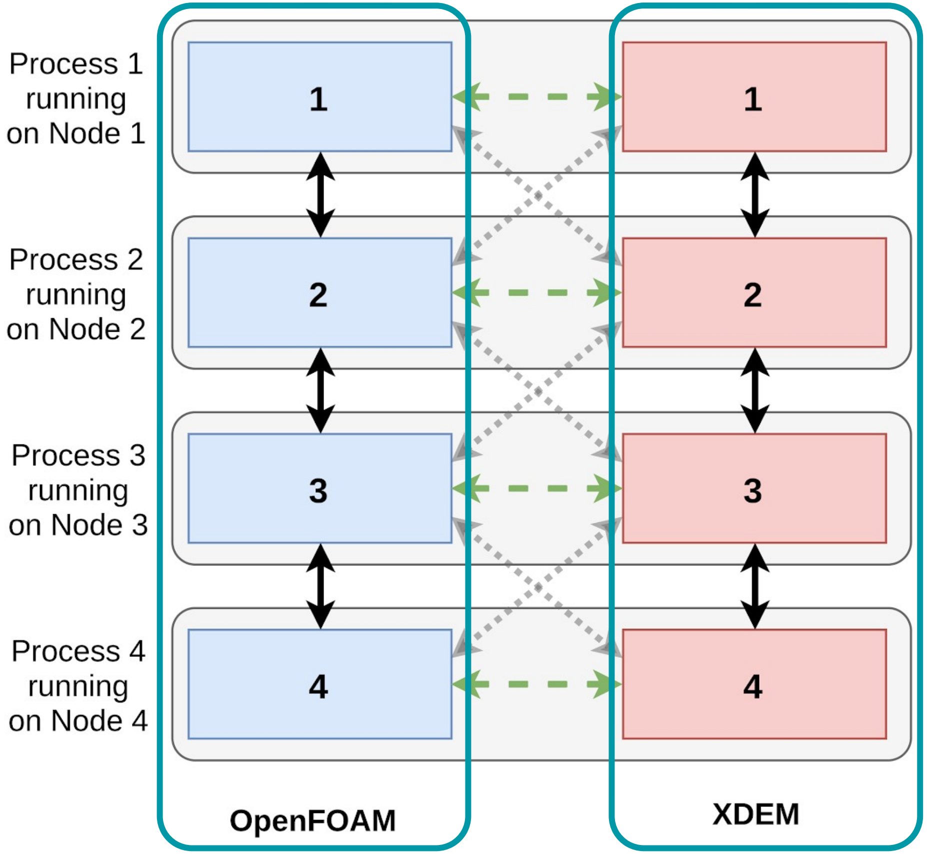
⟷ **Inter-partition intra-physics Data Exchange using MPI communication layer**
with native implementation in OpenFOAM and XDEM

Inter-physics Data Exchange

◁···▷ **Inter-partition inter-physics Data Exchange using MPI communication layer**
reduced to minimum or non-existing due to partition co-location

⇠ ⇢ **Intra-partition inter-physics Data Exchange using direct library function calls**
fast because it is a direct intra-process memory access

Co-located Partitioning Strategy: communication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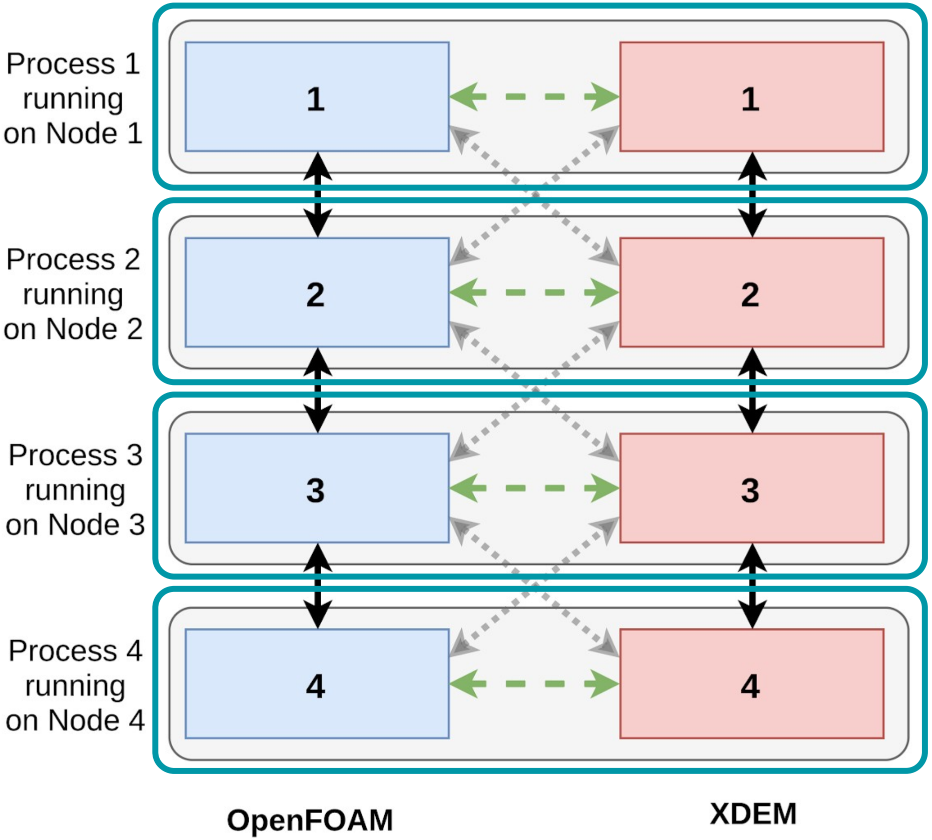
fast because it is a direct intra-process memory access

With native implementation of each sotfware

Co-located Partitioning Strategy: communication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Inter-physics Data Exchange

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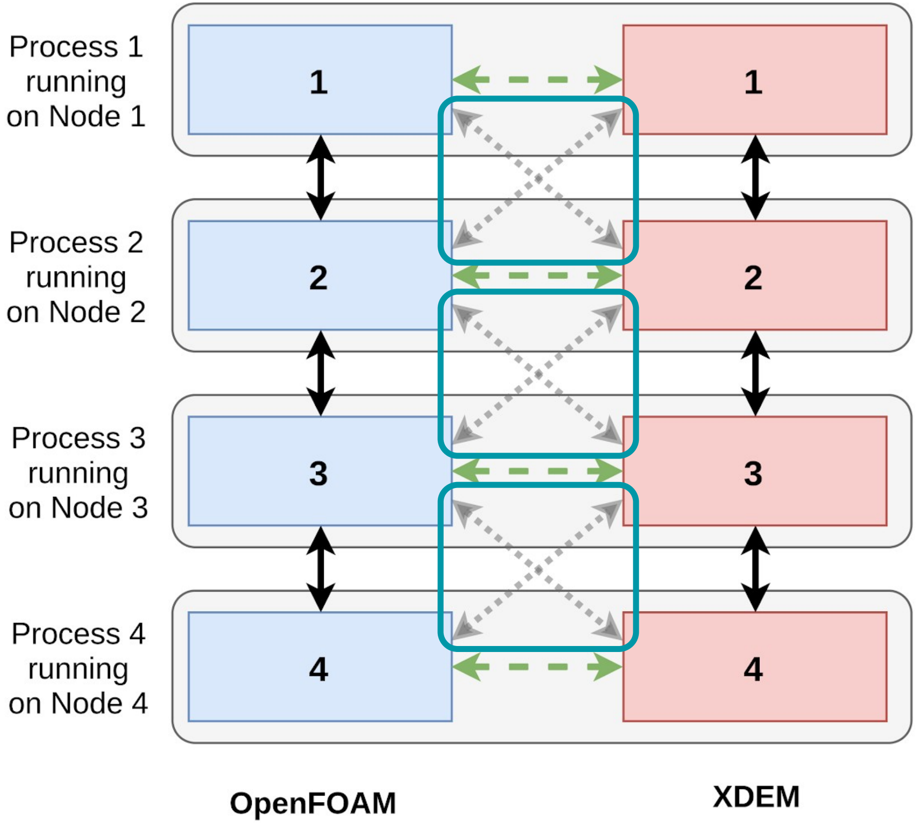
fast because it is a direct intra-process memory access

Use direct intra-proces memory access if the two software are linked into one executable,

Co-located Partitioning Strategy: communication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OpenFOAM
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Inter-physics Data Exchange

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reduced to minimum or non-existing due to partition co-location

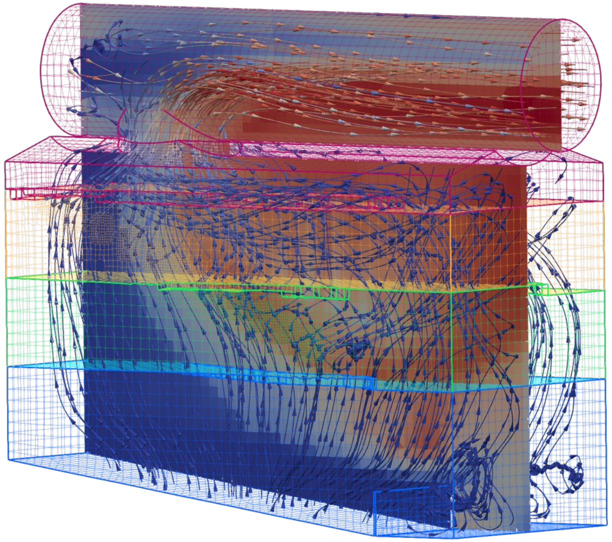
⇠ - ⇢ **Intra-partition inter-physics Data Exchange using direct library function calls**
fast because it is a direct intra-process memory access

**Can be non-existing
if partitions are perfectly aligned**

Volume Coupling for Biomass Furnace Simulation
Momentum, Heat and Mass transfer

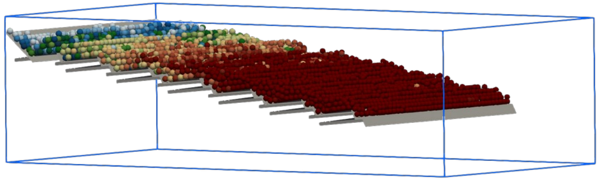
CFD to DEM

- Fluid *velocity*, density, dynamic viscosity
- *Pressure gradient*
- Temperature
- Thermal conductivity
- Specific heat
- Diffusivity
- Species mass fraction (CH4, CO2, CO, H2, H2O, N2, O2, Tar)



Fluid phase in OpenFOAM

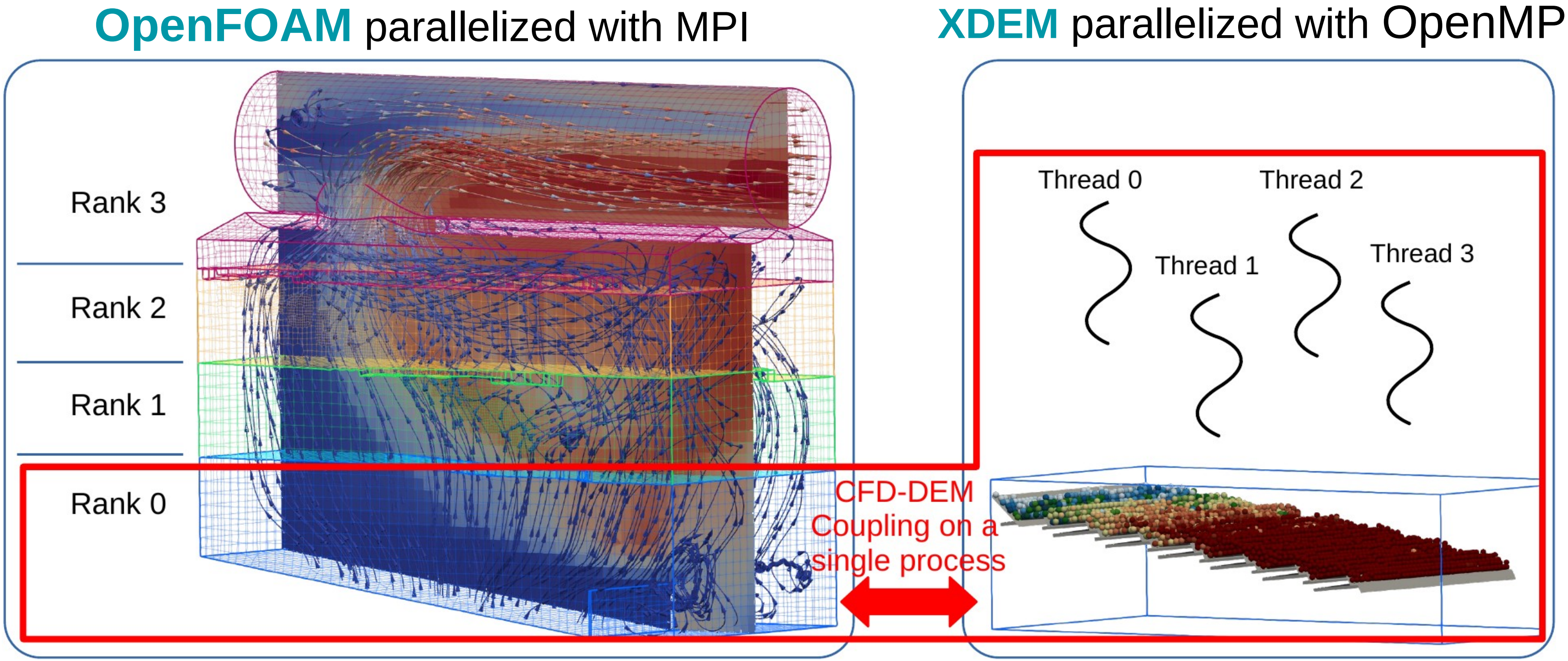
- Porosity
- Momentum source (*acceleration*, omega)
- Heat source
- Mass sources (CH4, CO2, CO, H2, H2O, N2, O2, Tar)



Particles in XDEM

DEM to CFD

Parallelization approach for Biomass Furnace Simulation


OpenFOAM parallelized with MPI
XDEM parallelized with OpenMP
Rank 3
Rank 2
Rank 1
Rank 0
Thread 0
Thread 2
Thread 1
Thread 3
CFD-DEM Coupling on a single process

Co-located partitioning → Account for the spatial-locality of the data between the two solvers

Overlapping domains are **co-located** ⇒ No inter-partition inter-physics communication

Solvers linked as one executable ⇒ Fast intra-partition inter-physics data exchange

Biomass Furnace Setup

based on an experimental furnace at Enerstena UAB in Lithuania

Furnace

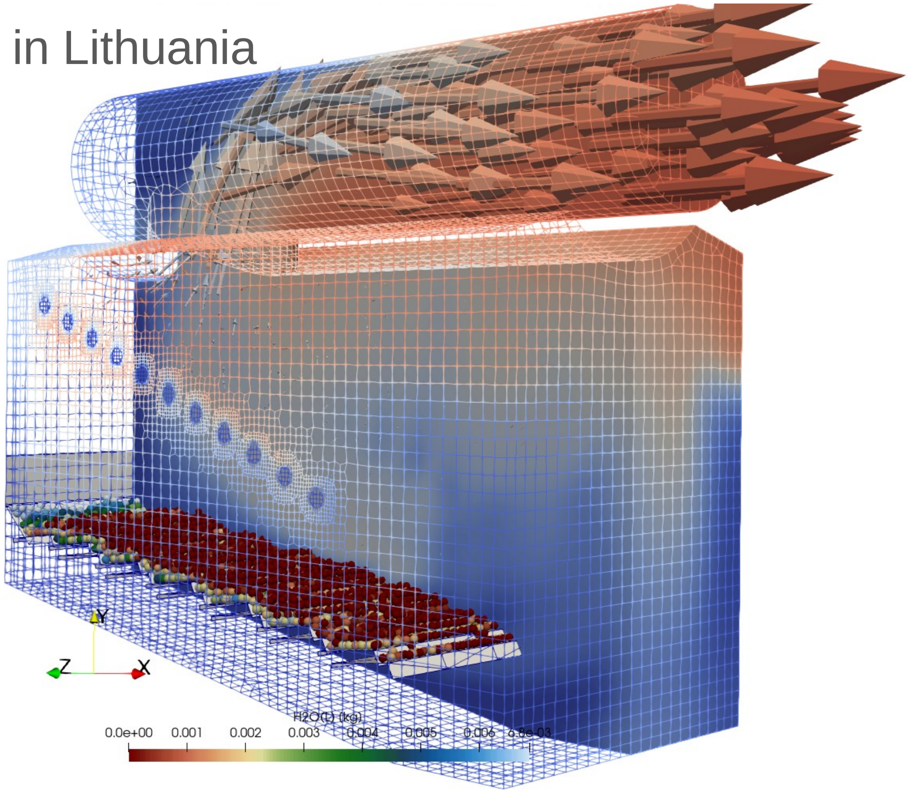
- Dimensions of 2.51m × 1.14m × 2.07m (L × W × H)
- Top exhaust pipe of 0.6m diameter
- 6 primary air inlets from the bottom
- 11 secondary air inlets on each side
- 1 tertiary air inlet on the exhaust pipe

Grates

- 8 static grates and
- 6 moving grates with an
- average slope of 7.5 degrees

Fuel bed

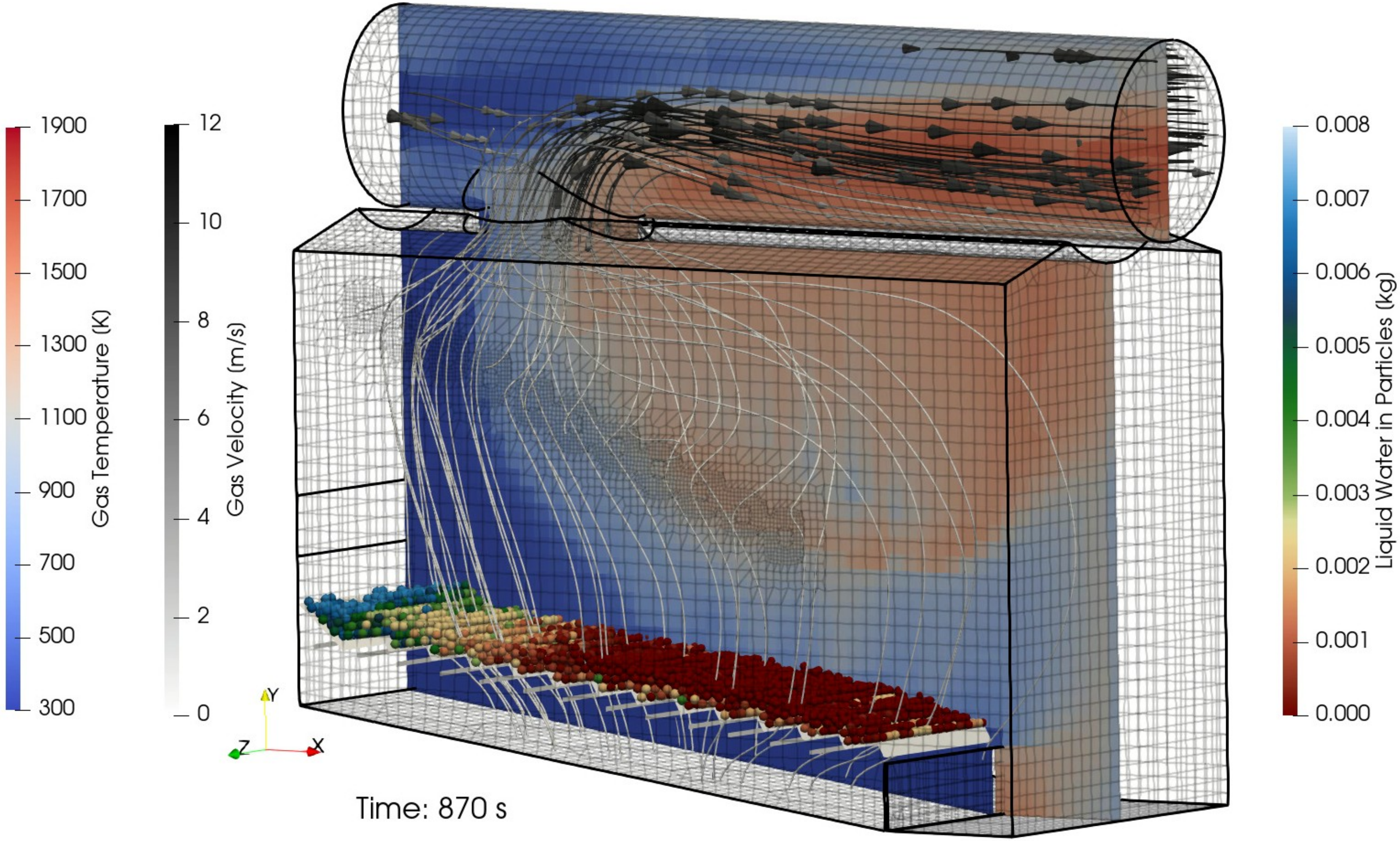
- Initial fuel bed height is 10cm
- Wood particles of 3cm diameter with 40% humidity
- Injected at the top side of the grates at a rate of 439kg/h



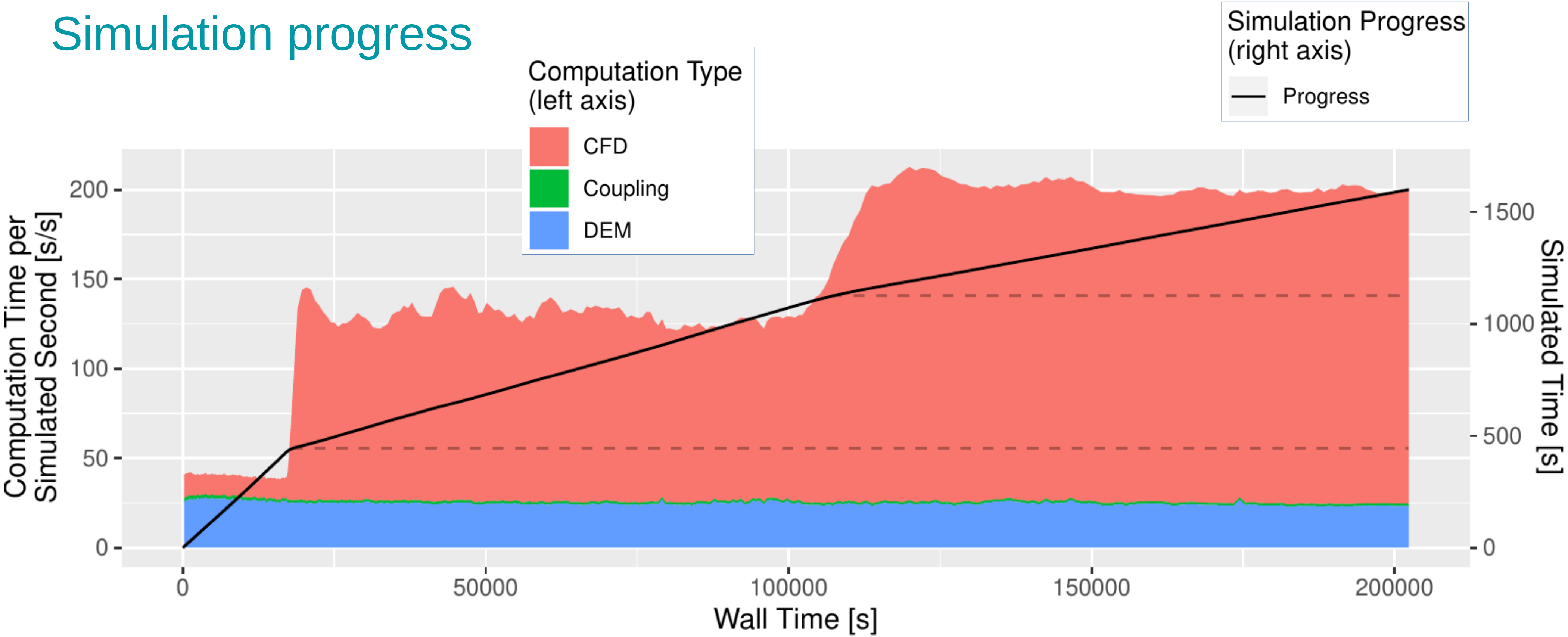
- CFD mesh with 60,001 cells
- 9,141 particles initially

Following performance measurements were carried out on the *Barbora* cluster of the IT4Innovations HPC platform.

Biomass Furnace simulation using XDEM+OpenFOAM



Simulation progress



- At 445s of simulated time, lighting-up of the furnace
- Around 1125s, furnace reaches the steady state (all hot gases are burning)

⇒ Workload between CFD and DEM changes with the simulation progress

References

References on HPC, Distributed Parallel Programming

The Free Lunch Is Over: A Fundamental Turn Toward Concurrency in Software
Herb Sutter, Dr. Dobb's Journal, 30(3), 2005. http://www.gotw.ca/publications/concurrency-ddj.htm

Designing and Building Parallel Programs: Concepts and Tools for Parallel Software Engineering
Ian Foster, 1995. https://www.mcs.anl.gov/~itf/dbpp/

Modern Operating Systems, Andrew Tanenbaum, 1992.

The Art of High Performance Computing, Victor Eijkhout, updated in 2022, https://theartofhpc.com/
- Volume 1: **Introduction to High-Performance Scientific Computing**
- Volume 2: **Parallel Programming for Science and Engineering**
- Volume 3: **Introduction Scientific Programming in Modern C++ and Fortran**

Using MPI: Portable Parallel Programming with the Message Passing Interface
Gropp et al., 2014. https://mitpress.mit.edu/books/using-mpi-third-edition

MPI Standard. https://www.mpi-forum.org/docs/
OpenMP Specifications. https://www.openmp.org/specifications/

Tools to work with the Roofline Model

CS Roofline Toolkit, Berkeley Lab
https://bitbucket.org/berkeleylab/cs-roofline-toolkit/

LIKWID, RRZE-HPC
https://github.com/RRZE-HPC/likwid

Intel Advisor, Intel
https://software.intel.com/en-us/advisor

References on the Roofline Model

Roofline: An Insightful Visual Performance Model for Multicore Architectures
Williams et al., CACM, 2009. DOI: 10.1145/1498765.1498785

Performance Tuning of Scientific Codes with the Roofline Model, Williams et al., SC'18 Tutorial, 2018
https://crd.lbl.gov/assets/Uploads/SC18-Roofline-1-intro.pdf

Applying the roofline model, Ofenbeck et al., ISPASS, 2014
DOI: 10.1109/ISPASS.2014.6844463

References on HPC for XDEM

Parallel Multi-Physics Simulation of Biomass Furnace and Cloud-based Workflow for SMEs
Besseron et al. PEARC’22, 2022. DOI: 10.1145/3491418.3530294

Large Scale Parallel Simulation For Extended Discrete Element Method
Mainassara Chekaraou A. W., PhD Thesis, 2020. http://hdl.handle.net/10993/46418

Predicting near-optimal skin distance in Verlet buffer approach for Discrete Element Method
Mainassara Chekaraou et al., PDCO’20, 2020. DOI: 10.1109/IPDPSW50202.2020.00093

A parallel dual-grid multiscale approach to CFD-DEM couplings
Pozzetti et al., Journal of Computational Physics, 2019. DOI: 10.1016/j.jcp.2018.11.030

The XDEM Multi-physics and Multi-scale Simulation Technology: Review on DEM-CFD Coupling, Methodology and Engineering Applications, Peters et al., Particuology, 2019. DOI: 10.1016/j.partic.2018.04.005

Hybrid MPI+OpenMP Implementation of eXtended Discrete Element Method
Mainassara Chekaraou et al., WAMCA’18. DOI: 10.1109/CAHPC.2018.8645880

Unified Design for Parallel Execution of Coupled Simulations using the Discrete Particle Method
Besseron et al., PARENG’13, 2013. DOI:10.4203/ccp.101.49

Thank you for your attention !

Question?

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https://sc-camp.org

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