TASK-BASED PROGRAMMING MODELS FOR SCALABLE ALGORITHMS

Application to matrix multiplication

Antoine Jego

November 6, 2022

Quick presentation

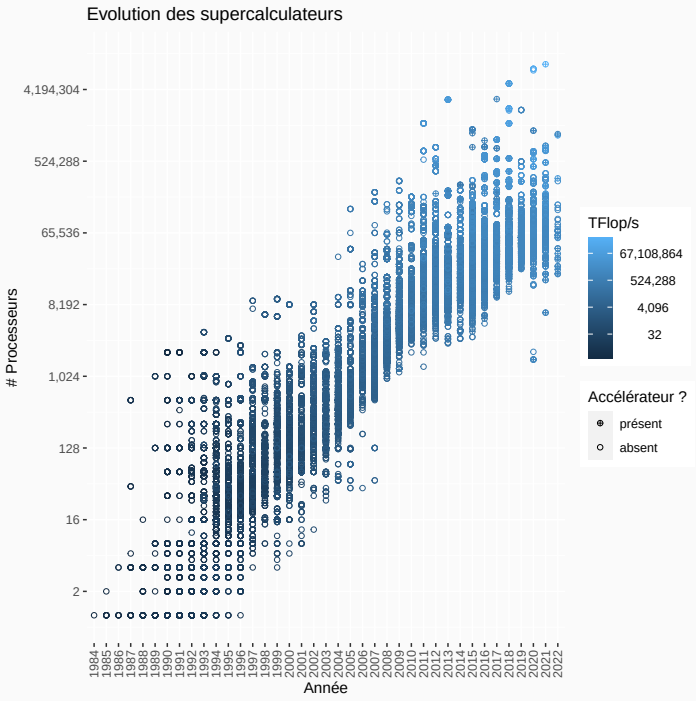
- 2019-2020: Finishing my engineering degree in ENSEEIHT ("HPC & Big Data")
  - My PFE was done in ENSEEIHT laboratory to quickstart the Phd Thesis

- 2020-2022 : 2 years as a PhD student
  - Collaborating with researchers from Bordeaux, Lyon, Toulouse as part of the SOLHARIS ANR project.

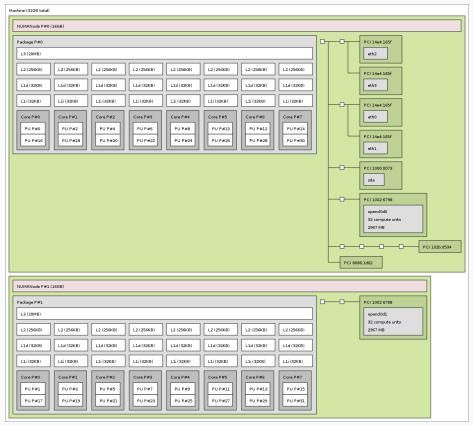
INTRODUCTION

Algorithms, architectures and programming models

Architectures are becoming increasingly **large**, **heterogeneous** and **complex**.



- Architecture
  - Single core 60s
  - Vectorized 70s
  - Multinode 90s
  - Multicore 00s
  - Accelerated 10s
- Software
  - Fortran '55
  - C '72
  - MPI '92
  - OpenMP '97
  - CUDA '07



A typical node architecture, with two multiple cores CPUs and two GPUs

Algorithms, architectures and programming models

Architectures are becoming increasingly **large**, **heterogeneous** and **complex**.

- Algorithms have to handle communications to achieve high scalability
  - Communication/computation overlap
  - Communication-avoiding algorithms

- Software should deliver a reliable abstraction to build mathematical software
  - parallel programming models
  - runtime systems

Are currently available parallel programming models and runtimes expressive enough to implement scalable algorithms in an efficient, portable and maintainable way?

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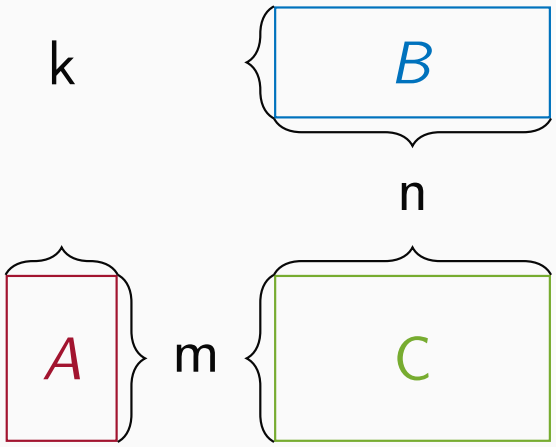
Algorithms, architectures and programming models

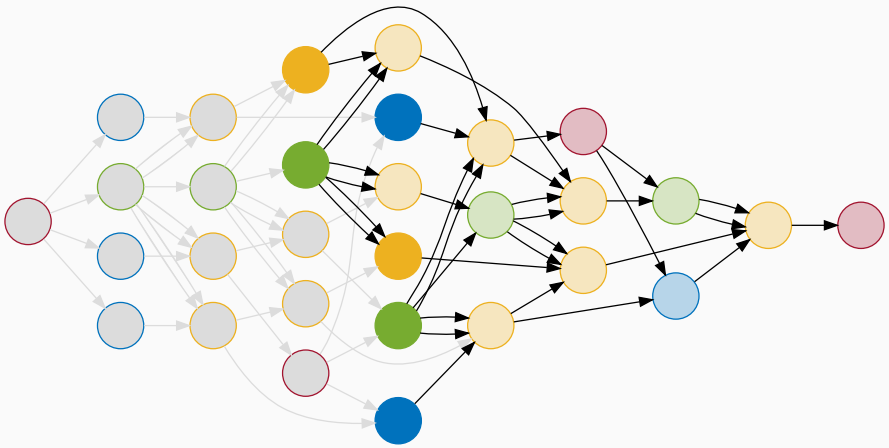
We take the following examples to answer this large question

- Algorithms: scalable dense matrix multiplication (GEMM) algorithms such as SUMMA and 2.5D SUMMA

$$C = \alpha AB + \beta C$$



- Software: task-based parallel programming paradigm through the sequential task flow (STF) model



BACKGROUND

Generalities

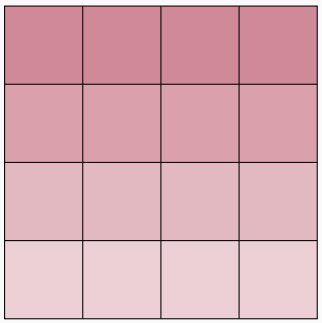
We focus on $C = AB$. Matrices are partitioned by blocks.

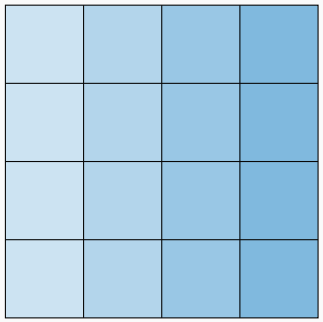
For each block $C_{i,j}$ of C, we compute $C_{i,j} = \sum_{l=1}^{k} A_{i,l} B_{l,j}$.
Each contribution $A_{i,l} B_{l,j}$ is identified as $T_{i,j,l}$ in a tensor T.

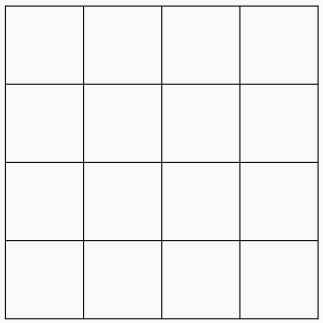
Algorithms for GEMM have to

- state an initial data distribution
- state what process handles $T_{i,j,l}$
- state how blocks are exchanged
- state a final distribution

Distributed-memory GEMM Algorithms







Cannon algorithm

- **Data mapping**
  - 2D block
- **Workload mapping**
  - owner of C computes
- **Communications**
  - initial row-wise skew of A
  - initial column-wise skew of B
  - row-wise circular shift of A
  - column-wise circular shift of B

```
! I am r × c
send_recv(A, mod(r+c,n)×mod(r+c,n))
send_recv(B, mod(r+c,n)×mod(r+c,n))
do l=range(1,n).sort_first(mod(r+c),n)
   call gemm(A, B, C_{r,c})
   send_recv(A, mod(r+1,p)×c)
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end do
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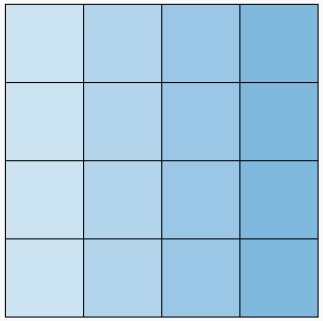
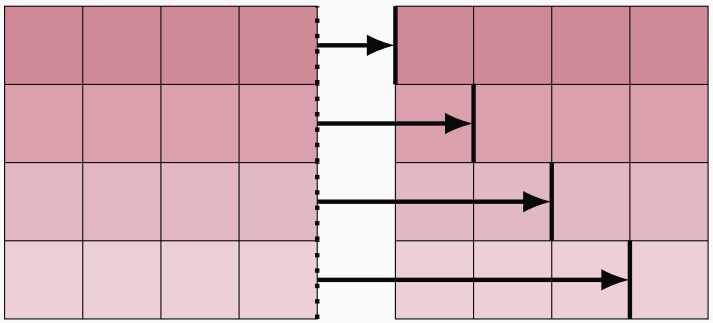
Cannon, 1969

Distributed-memory GEMM Algorithms





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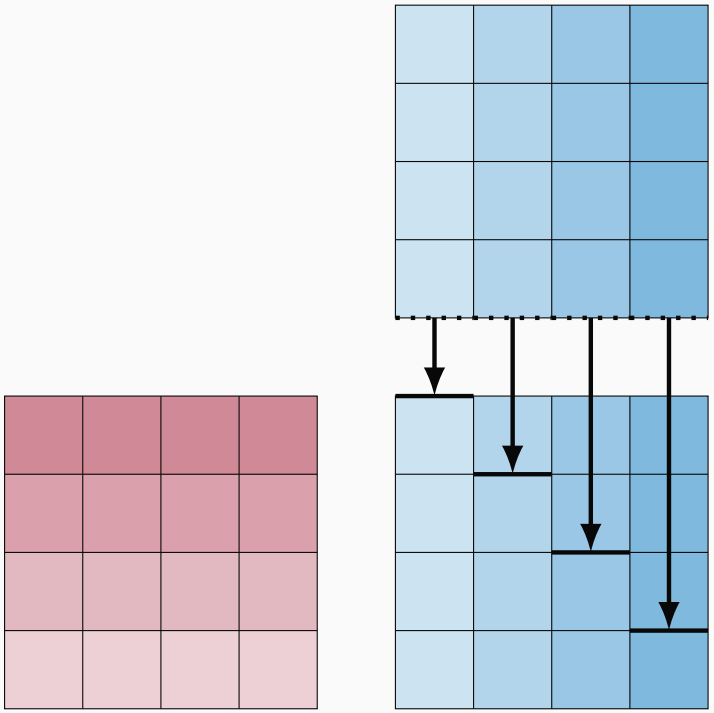

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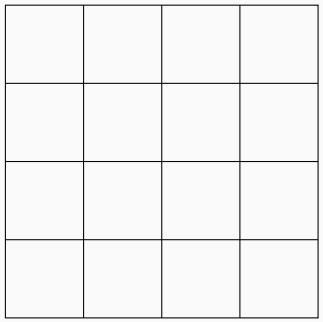

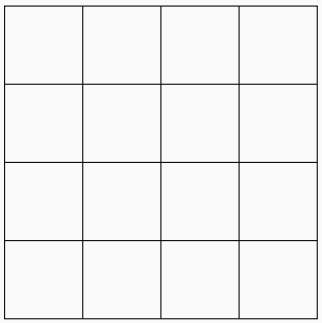

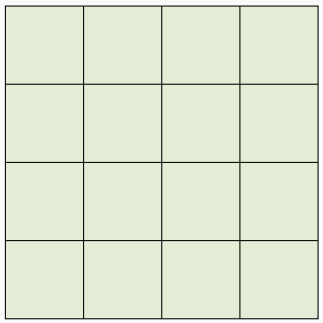

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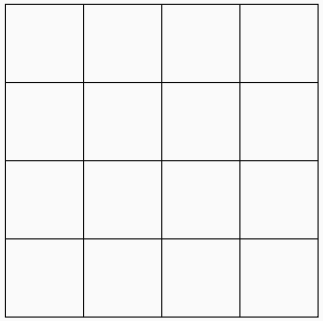

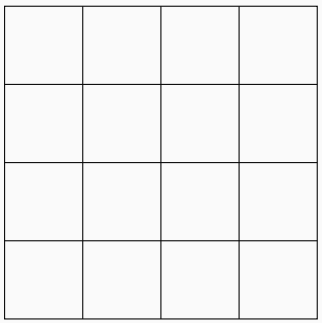

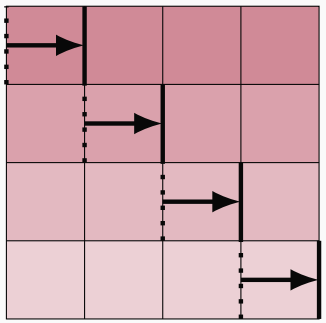

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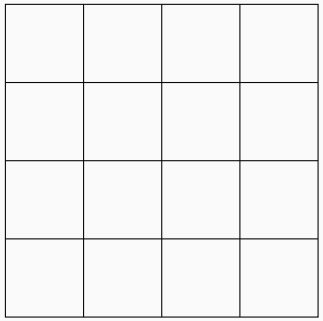

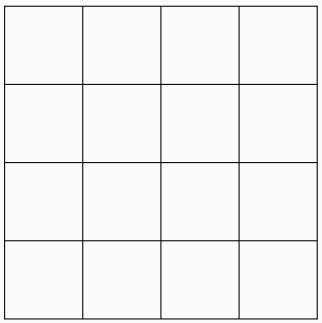

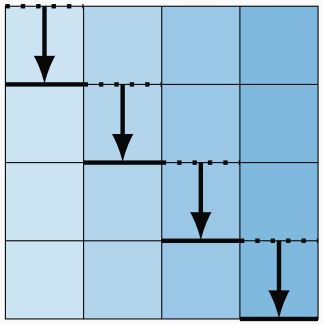

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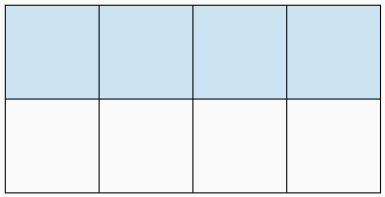

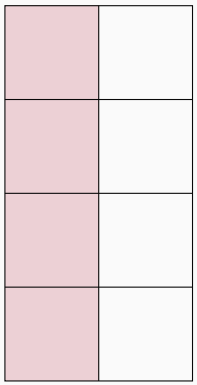

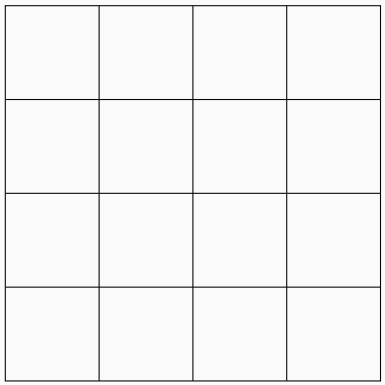

2D C-stationary SUMMA

- **Data mapping**
  - 2D block-cyclic
- **Workload mapping**
  - owner of C computes
- **Communications**
  - row-wise broadcast of A
  - column-wise broadcast of B

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do l=1, k
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Geijn and Watts, 1997

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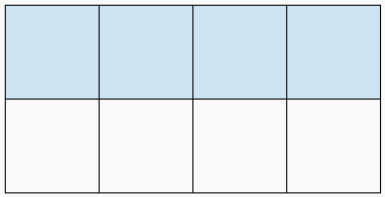

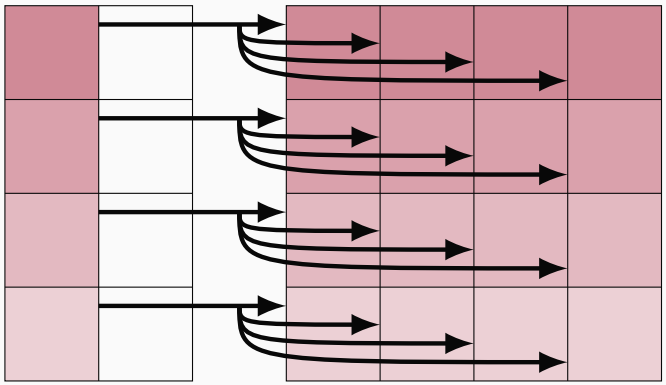

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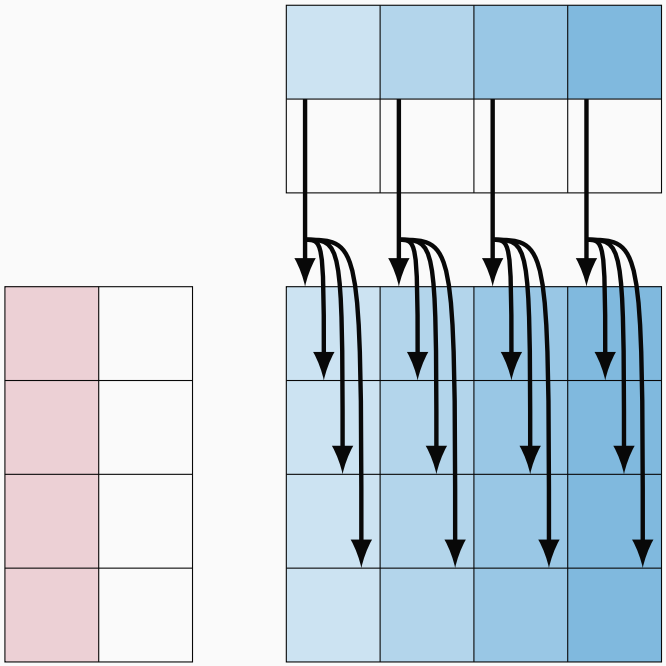

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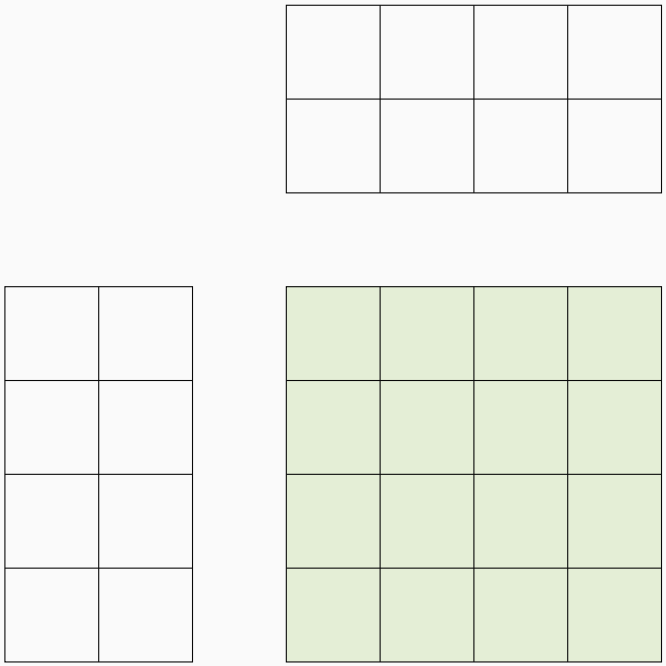

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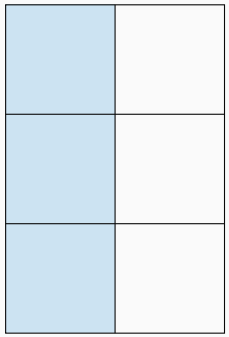

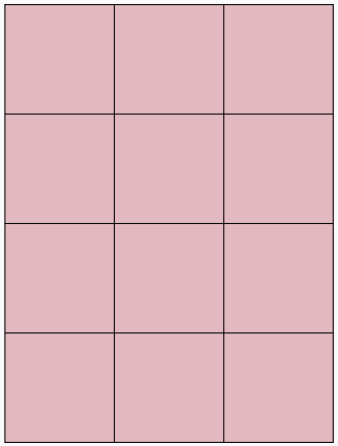

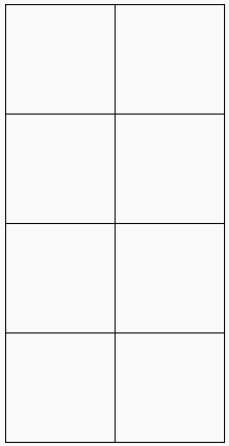

2D A-stationary SUMMA

- **Data mapping**
  - 2D block-cyclic
- **Worload mapping**
  - owner of A computes
- **Communications**
  - column-wise scatter+broadcast of B
  - row-wise reduction of C

```
! I am r × c
do j=1, n
   forall l, l%p==r.and.l%q==c :
      recv(B_{l,j}, l%p×j%q)
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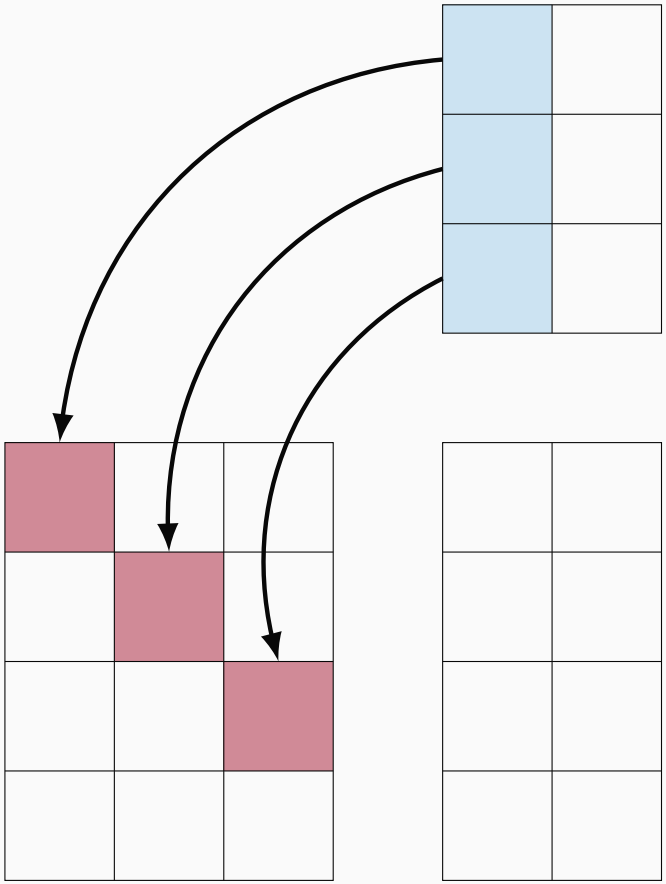
Geijn and Watts, 1997

Distributed-memory GEMM Algorithms



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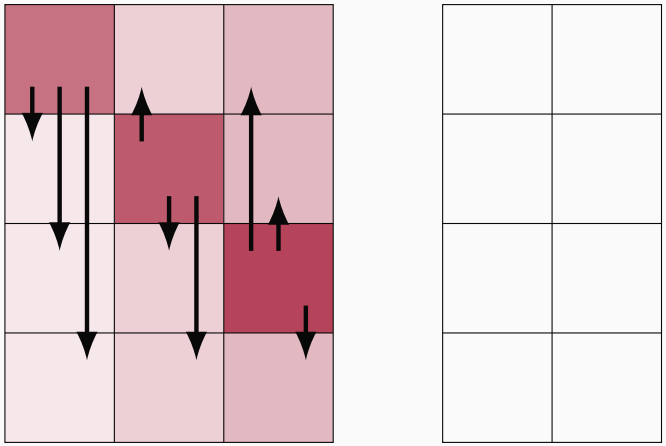

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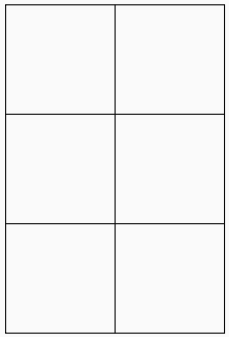
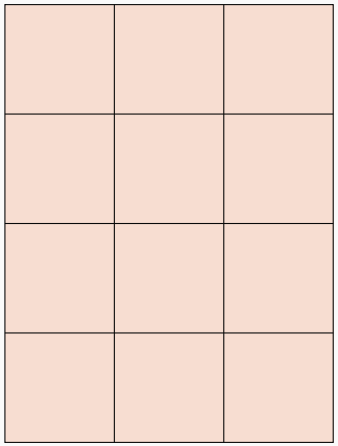
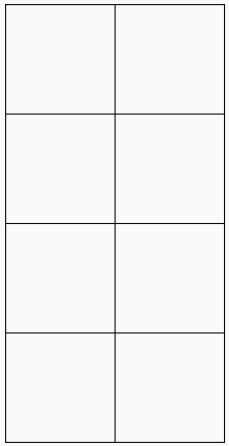
Distributed-memory GEMM Algorithms







2D A-stationary SUMMA

- **Data mapping**
  - 2D block-cyclic
- **Worload mapping**
  - owner of A **computes**
- **Communications**
  - column-wise scatter+broadcast of B
  - row-wise reduction of C

```
! I am r × c
do j=1, n
   forall l, l%p==r.and.l%q==c :
      recv(B_{l,j}, l%p×j%q)
   forall l, l%p==c :
      bcast(B_{l,j}, *×c)
   forall i, i%p==r :
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         call gemm(A_{i,l}, B_{l,j}, C_{i,j})
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```

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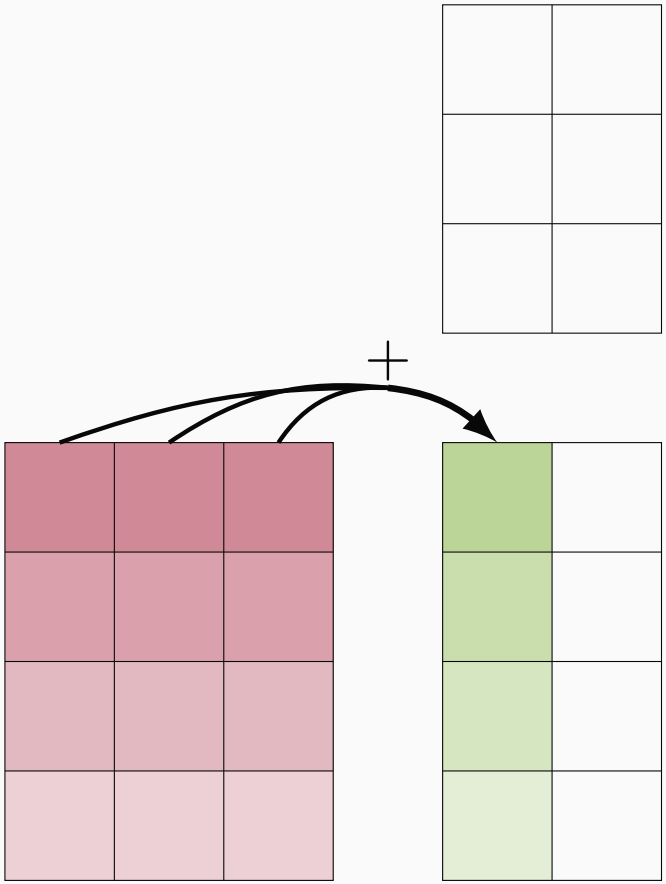

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Distributed-memory GEMM Algorithms

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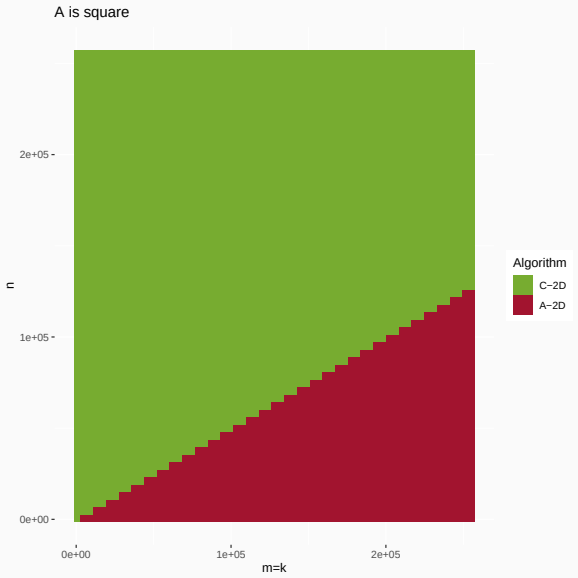
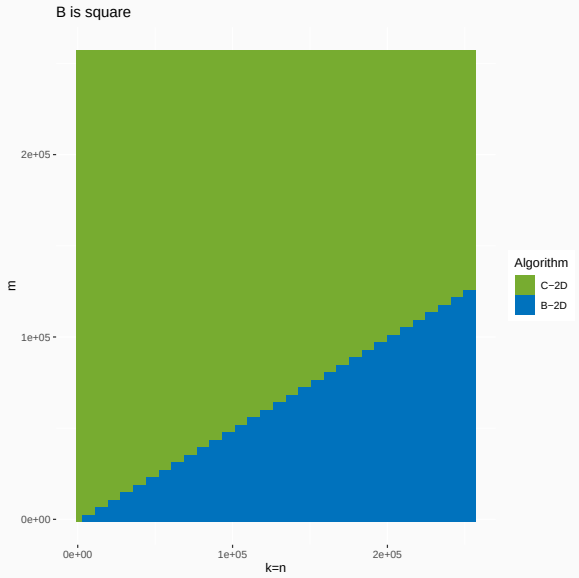
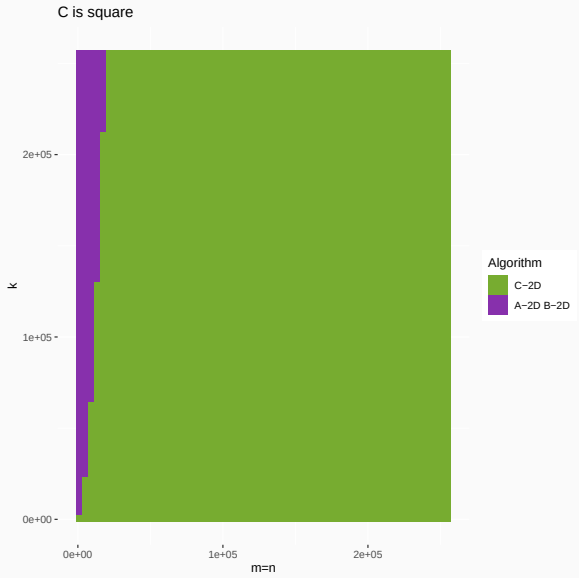
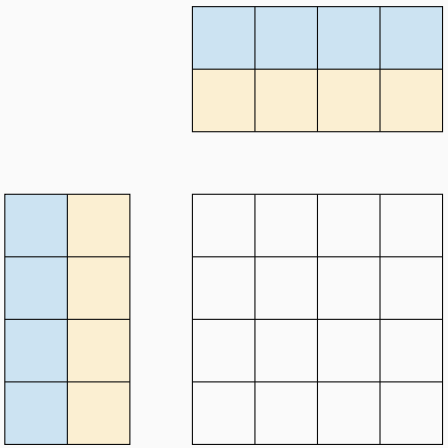




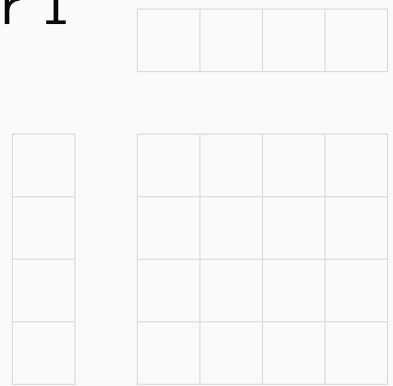


Distributed-memory GEMM Algorithms

Layer 0



Layer 1



2.5D C-stationary SUMMA

- **Data mapping**
  - 2D block-cyclic on 0^{th} layer
- **Workload mapping**
  - Not trivially related to data mapping
- **Communications**
  - row-wise scatter+broadcast of A
  - column-wise scatter+broadcast of B
  - aisle-wise reduction of C

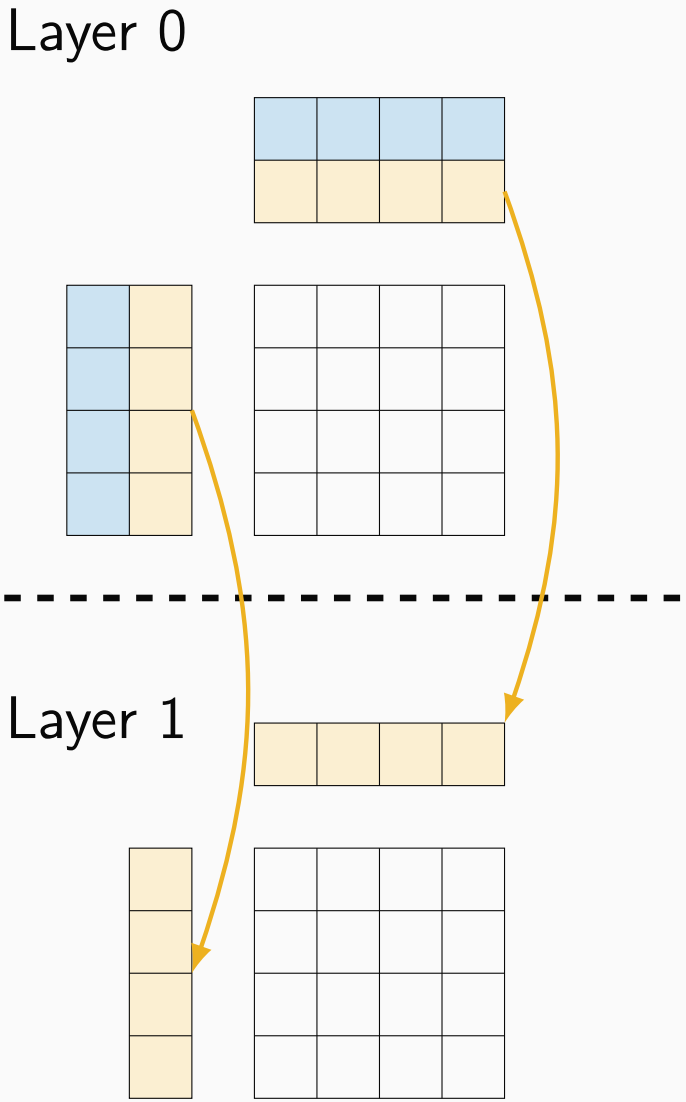
```
! I am r × c × h
scatter A_{i,j} on layer j/h
scatter B_{i,j} on layer i/h

forall layer=1,h:
   call SUMMA_2DC(A[:, (layer : layer + 1) * k/h],
                  B[(layer : layer + 1) * k/h, :], C^h)

forall i, i%p==r :
  forall j, j%q==c :
    reduce(C^h_{i,j}, r×c×0)
```

Irony, Toledo, and Tiskin, 2004

Distributed-memory GEMM Algorithms



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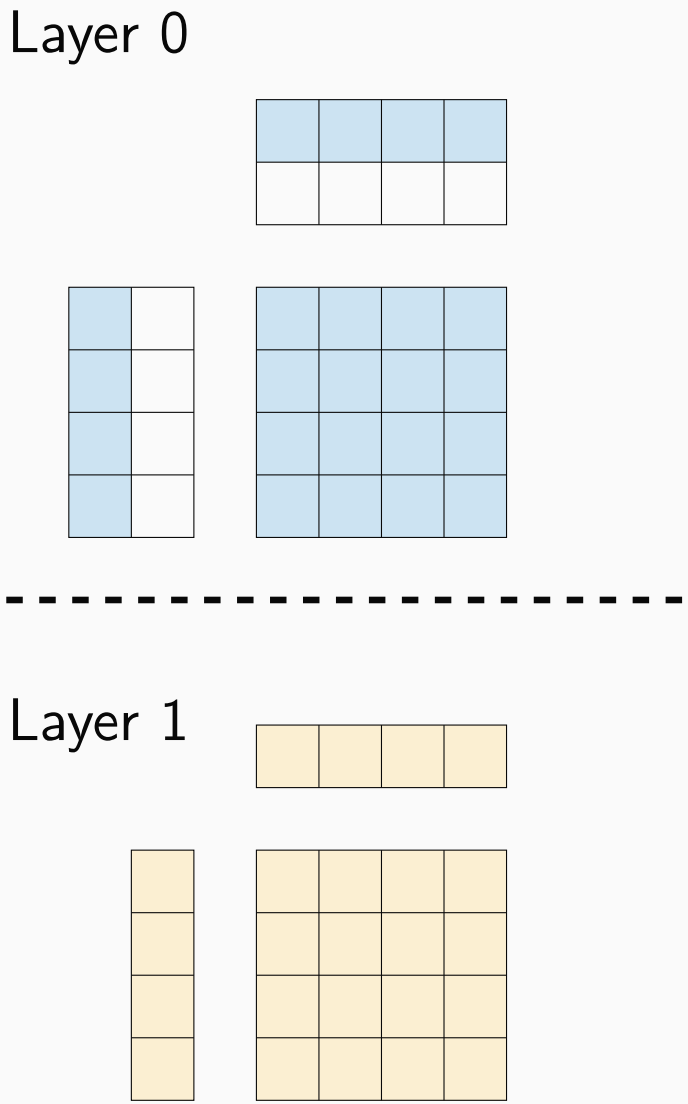

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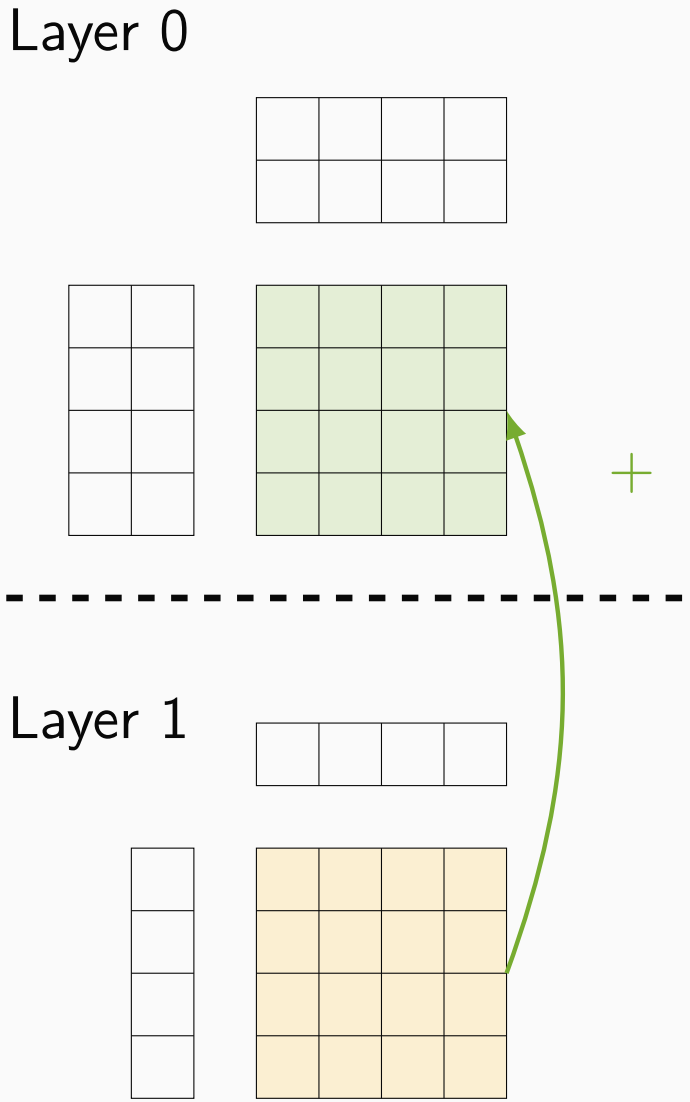

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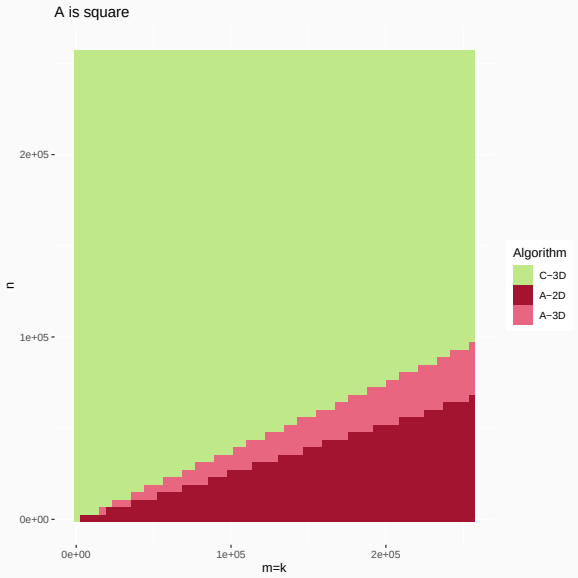
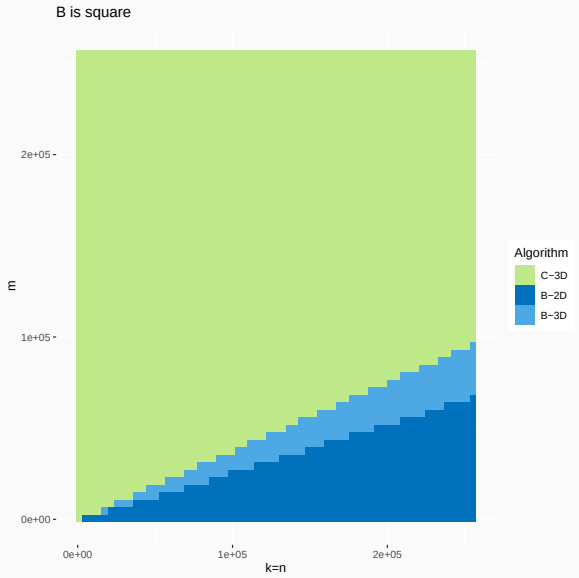
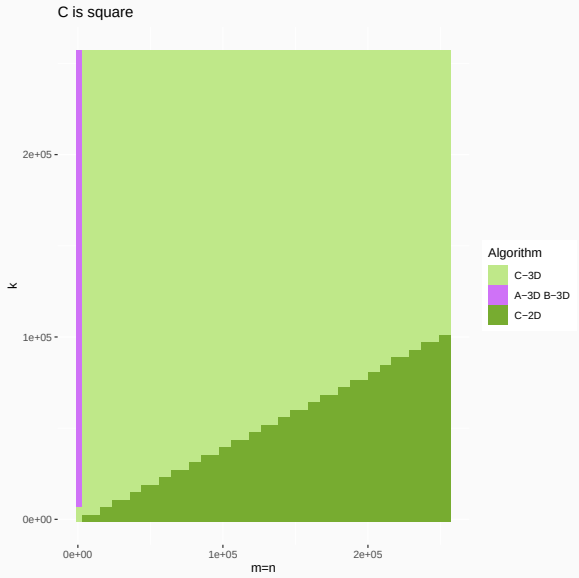
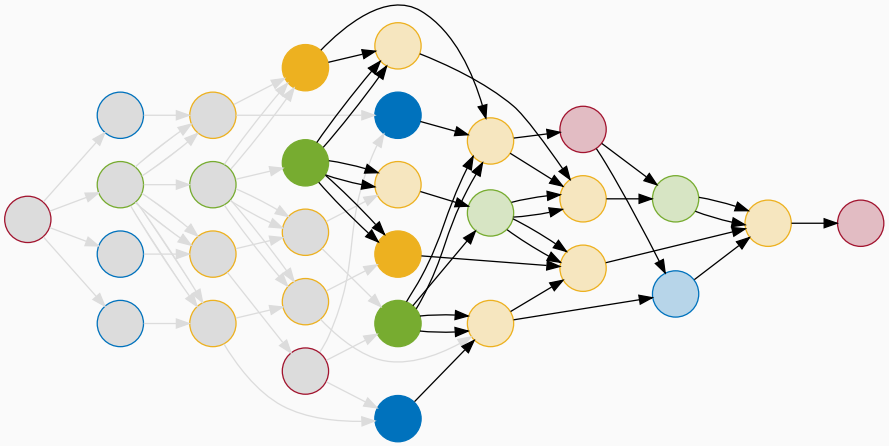






Task-based programming model



Directed acyclic graph (DAG)

- **Node** Elementary task
- **Edge** Dependencies between task

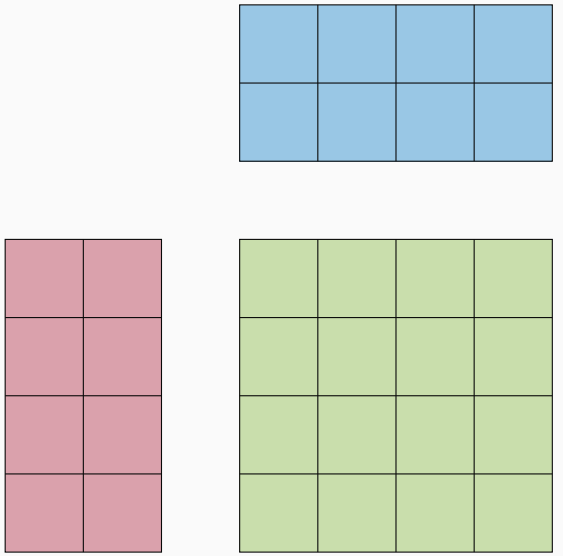
Several libraries expose a task-based programming model

- OpenMP (since 4.0)
- StarPU – developed in Bordeaux
- ParSEC
- ...

The sequential task flow (STF) Model

Sequential GEMM

```
do i=1,m
  do j=1,n
    do l=1,k
      call gemm(
                    A_{i,l},
                    B_{l,j},
                    C_{i,j} )
    end do
  end do
end do
```



Shared-memory STF GEMM

```
do i=1,m
  do j=1,n
    do l=1,k
      call insert_task( gemm,
                    A_{i,l}:R,
                    B_{l,j}:R,
                    C_{i,j}:RW)
    end do
  end do
end do
```


DAG of GEMM

The sequential task flow (STF) Model

Sequential GEMM

```
do i=1,m
  do j=1,n
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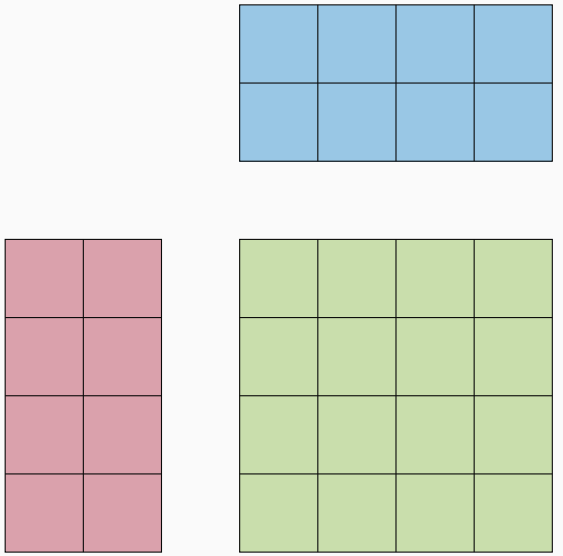

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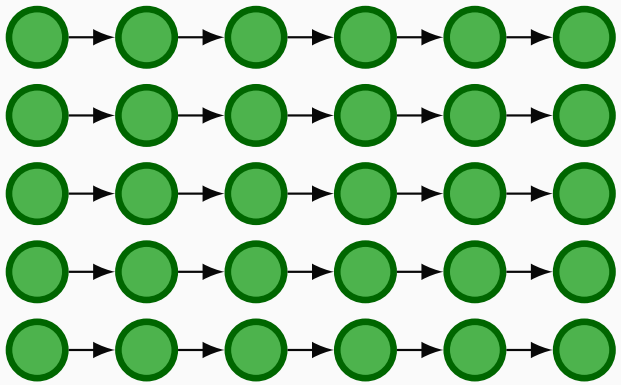

DAG of GEMM

Objectives

- Can we use the **STF model** to express a **scalable distributed-memory GEMM** algorithm ?

- How **efficient** is the resulting expression compared to reference libraries ?

DISTRIBUTED-MEMORY STF GEMM ALGORITHM

Baseline STF model

```
!
do i=1,m
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    do l=1,k
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    end do
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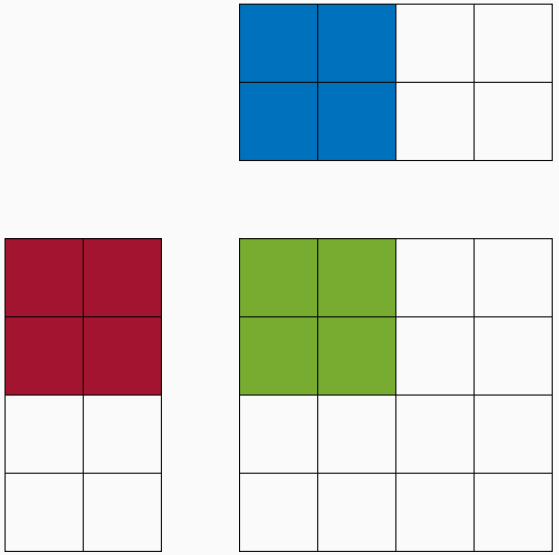
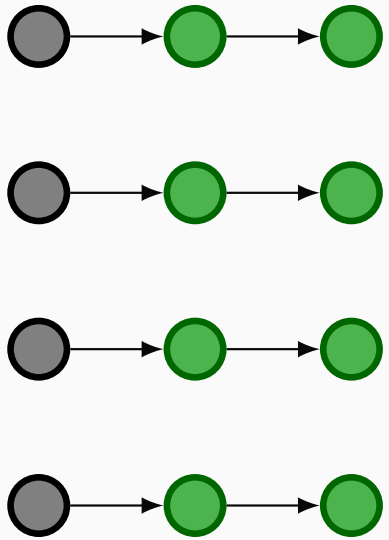


Baseline model (M0)[a]

- M0-0 Data mapping
- M0-1 Task mapping **inferred** from DM (RW)
- M0-2 Point-to-point comms. **inferred** from TM



[a] Agullo, Aumage, Faverge, Furmento, Pruvost, Sergent, and Thibault, 2017.

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```
! data_map: A,B,C distributed on a grid
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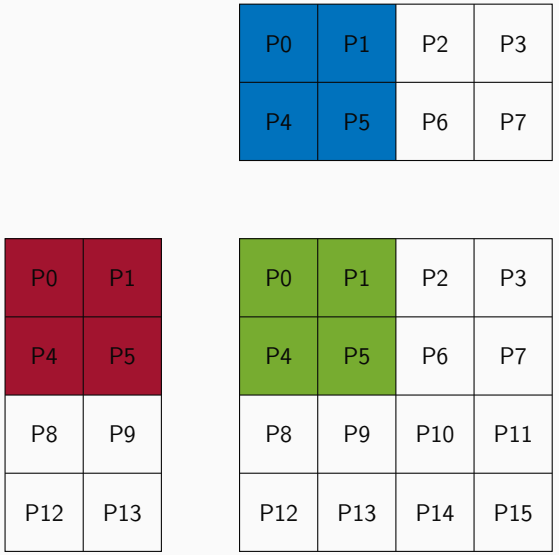

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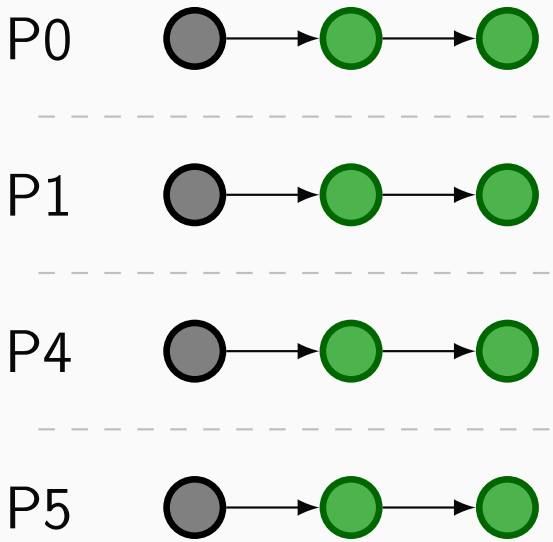

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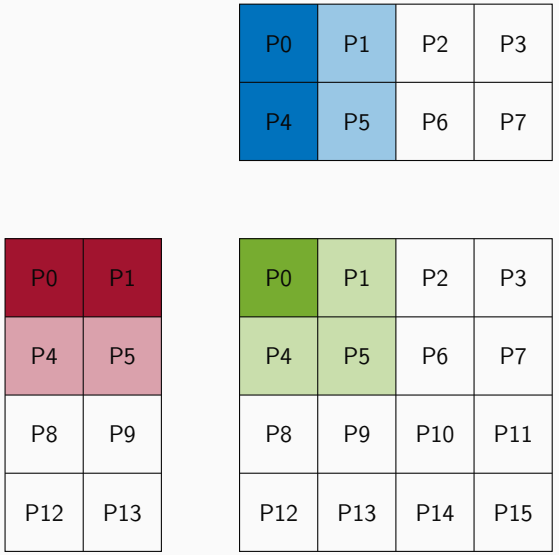

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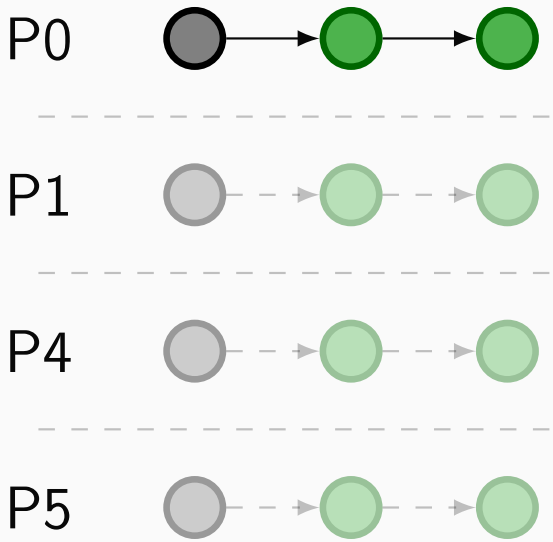

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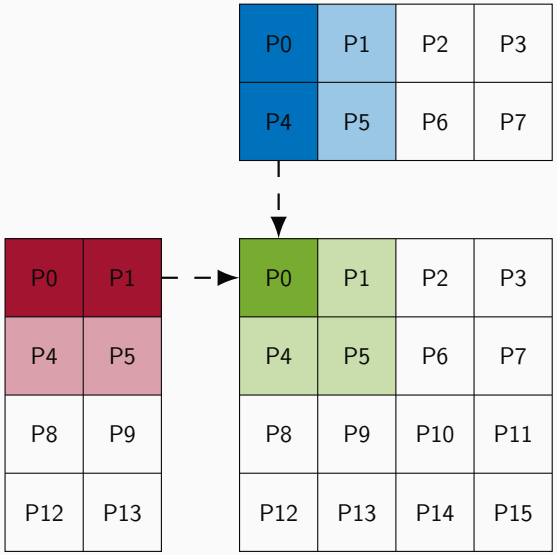

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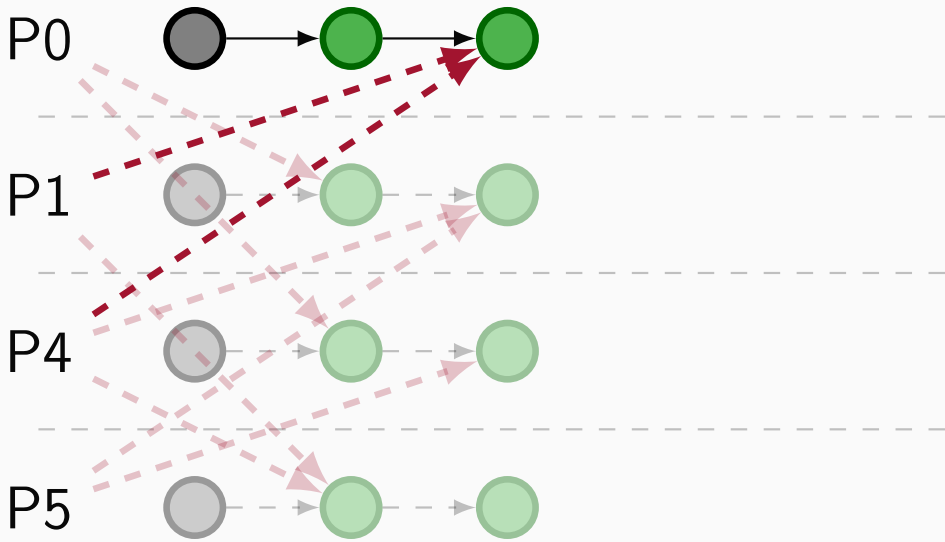

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Limits to the baseline model

The baseline STF model `M0` does not allow the expression of SUMMA algorithms

- Task mapping is bound to data mapping (`M0-1`)
- Reduction patterns are hard to make
- Point-to-point communications patterns are inefficient (`M0-2`)

We have identified key functionalities required in a STF model `MX`, extended from `M0`, to allow the expression of SUMMA algorithms.

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Key 1 – Task mapping

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!data_map: A,B,C distributed on one
      layer
!
!

do i=1,m
  do j=1,n
    do l=1,k
      call insert_task(gemm,
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    end do
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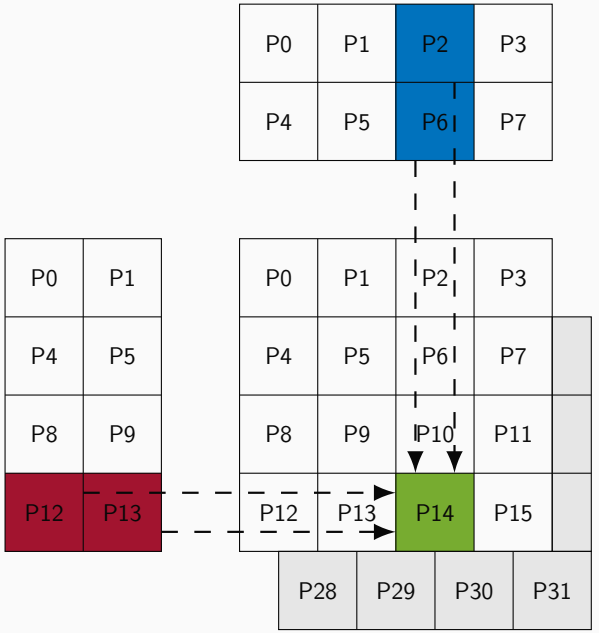
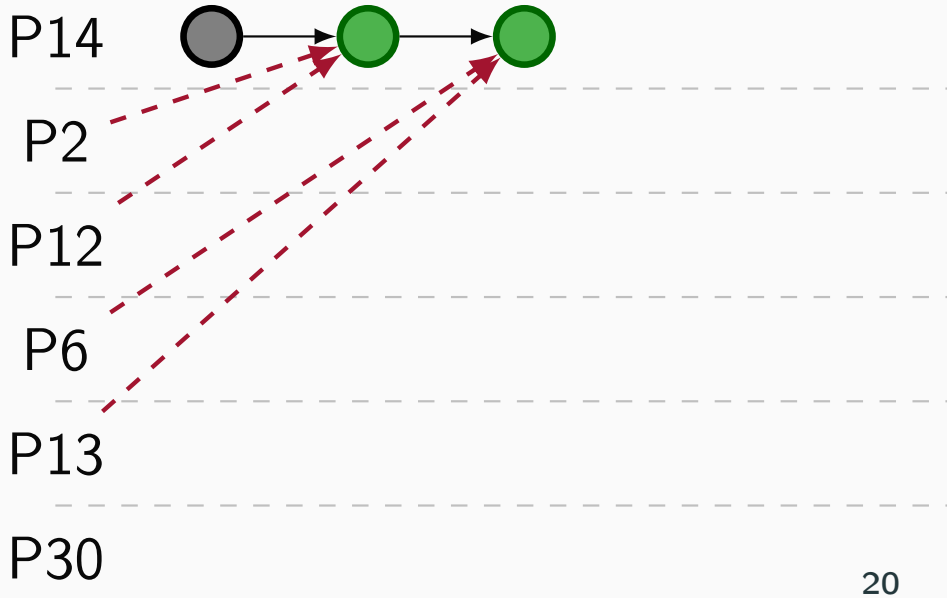


Advanced model MX

- M0-0 Data mapping
- M0-1 Implicit task mapping
- M0-2 Comms. inferred



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                       task_map[i,j,l])
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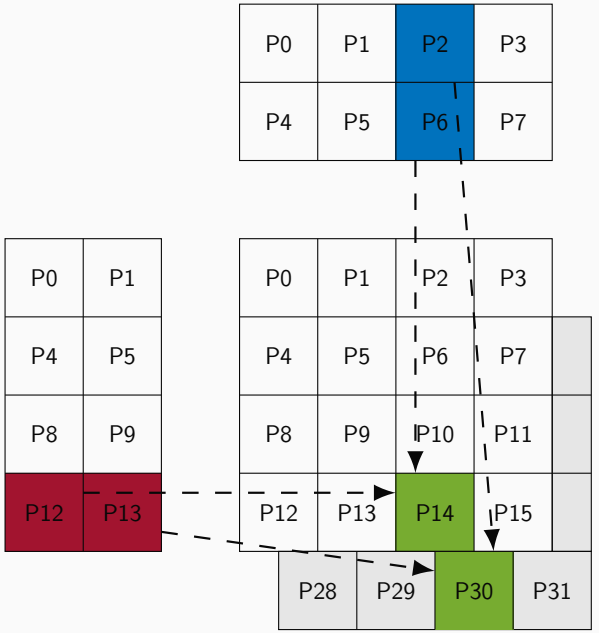

Advanced model MX

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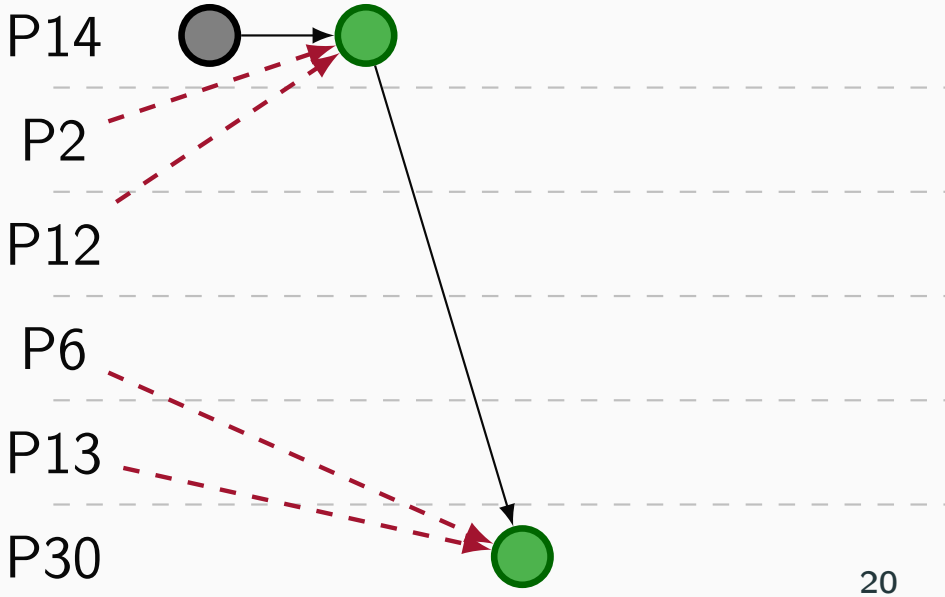
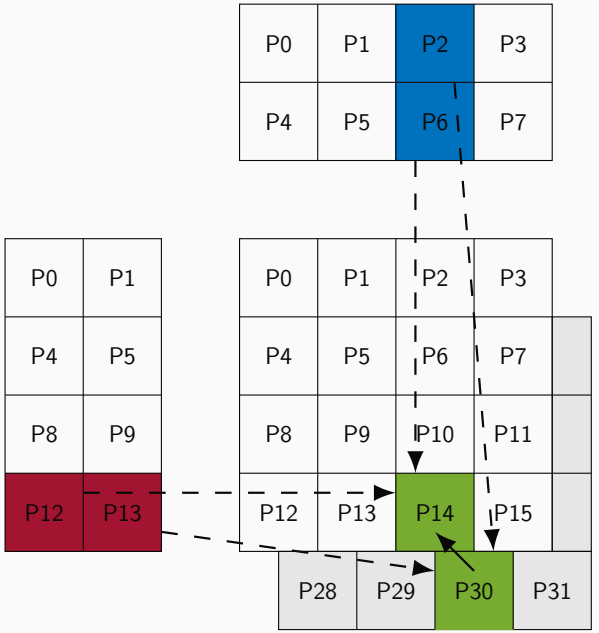


Key 2 – Reduction pattern

```
!data_map: A,B,C distributed on one
     layer
!task_map: executing node of A_{i,l}B_{l,j}
!
call instantiate_local(C)
do i=1,m
  do j=1,n
    do l=1,k
      call insert_task(gemm,
                       A_{i,l}:R,
                       B_{l,j}:R,
                       C_{i,j}:RW,
                       task_map[i,j,l])
    end do
  end do call reduce(C_{i,j})
end do
```



Advanced model MX

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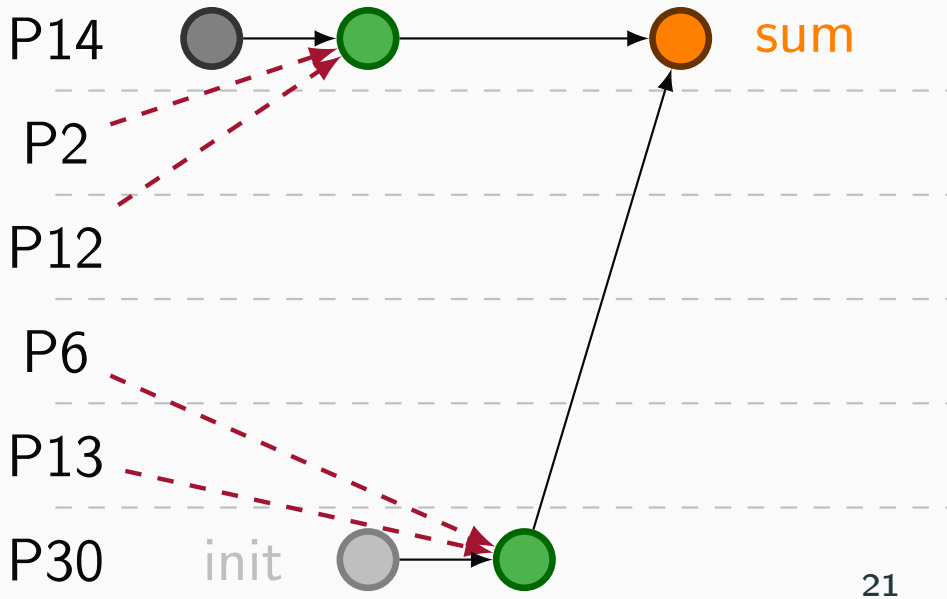
- MX-1 Explicit task mapping
- MO-2 Comms. inferred
- MO-3 Explicit reduction pattern



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    do l=1,k
      call insert_task(gemm,
                       A_{i,l}:R,
                       B_{l,j}:R,
                       C_{i,j}:RANK_REDUX,
                       task_map[i,j,l])
    end do
  end do call reduce(C_{i,j})
end do
```
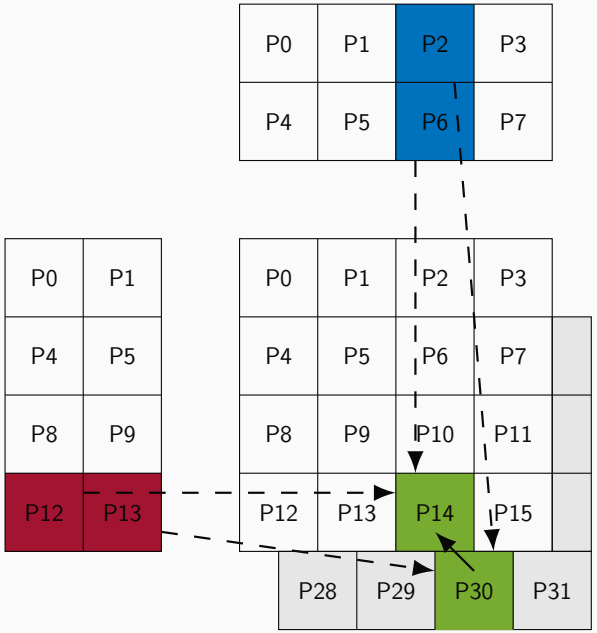
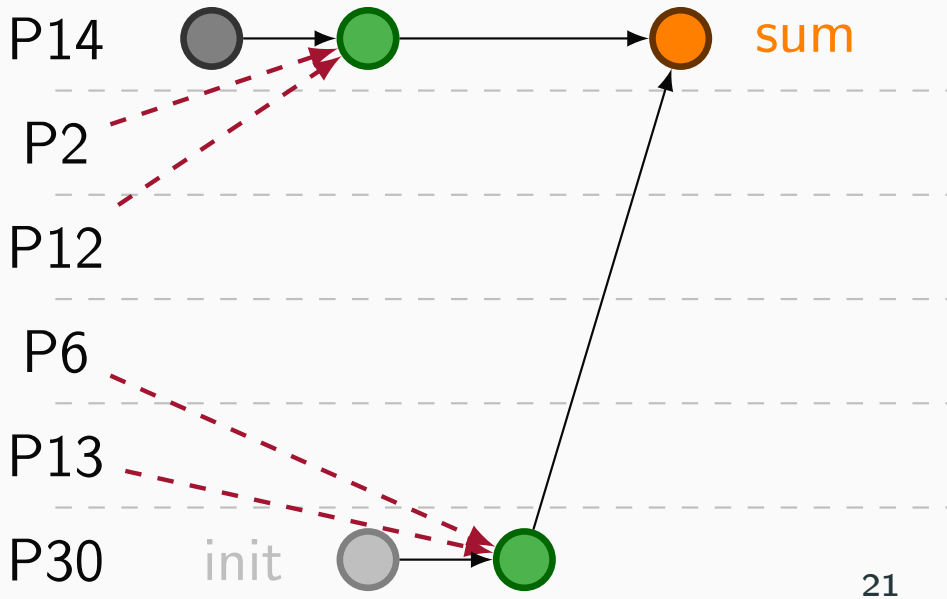



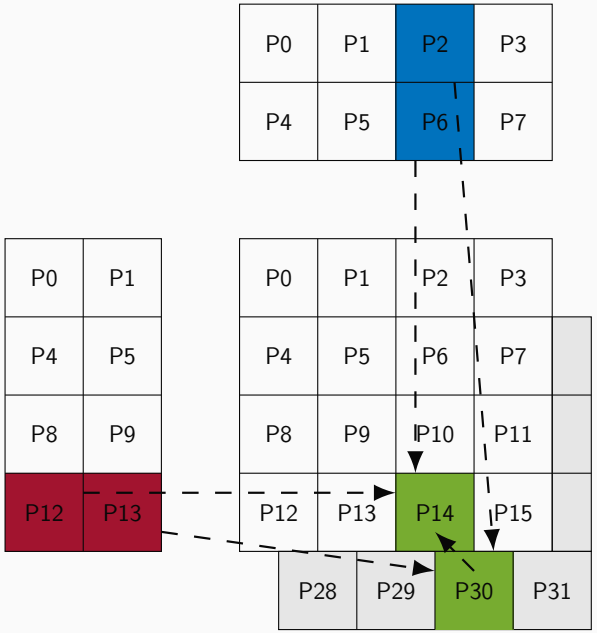
Advanced model MX

- MO-0 Data mapping
- MX-1 Explicit task mapping
- MO-2 Comms. inferred
- MO-3 Explicit reduction pattern



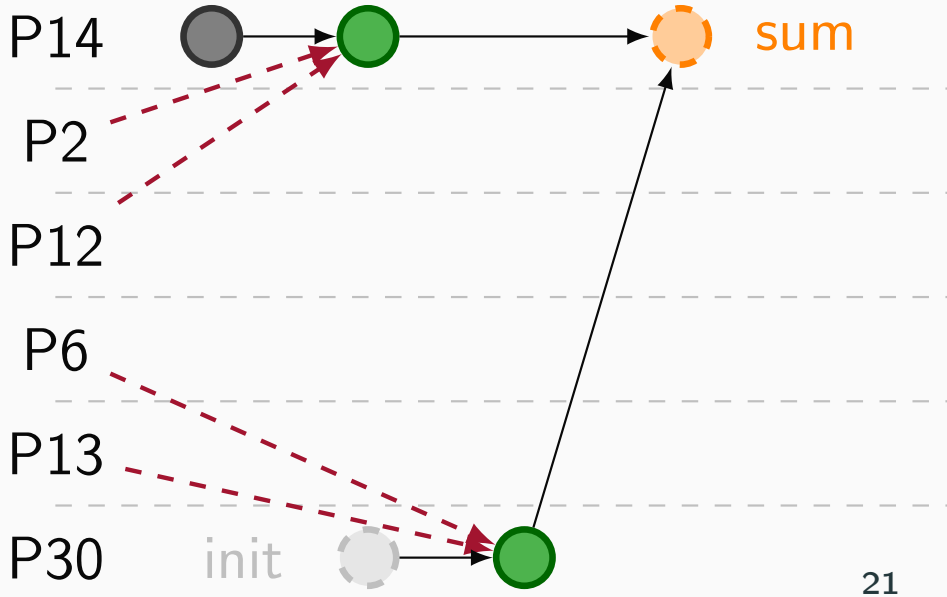
Key 2 – Reduction pattern

```
!data_map: A,B,C distributed on one
     layer
!task_map: executing node of A_{i,l}B_{l,j}
!
call bind_methods(C, init, sum)
do i=1,m
  do j=1,n
    do l=1,k
      call insert_task(gemm,
                       A_{i,l}:R,
                       B_{l,j}:R,
                       C_{i,j}:RANK_REDUX,
                       task_map[i,j,l])
    end do
  end do
end do
```



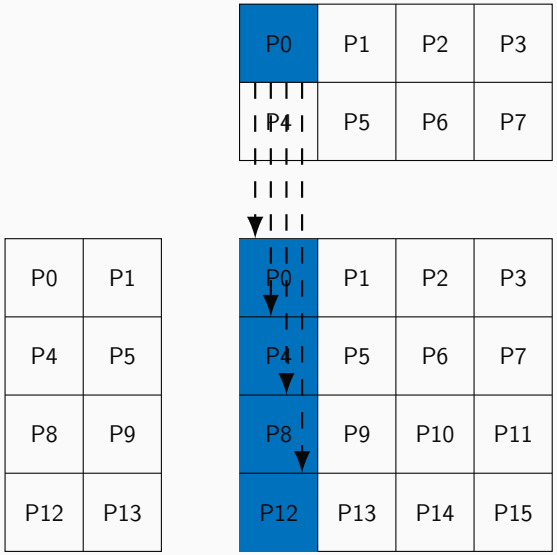
Advanced model MX

- MO-0 Data mapping
- MX-1 Explicit task mapping
- MO-2 Comms. inferred
- MX-3 **Implicit** reduction pattern



Key 3 – Communications

```
!data_map: A,B,C distributed on one
     layer
!task_map: executing node of A_{i,l}B_{l,j}
!
call bind_methods(C, init, sum)
do i=1,m
  do j=1,n
    do l=1,k
      call insert_task(gemm,
                       A_{i,l}:R,
                       B_{l,j}:R,
                       C_{i,j}:RANK_REDUX,
                       task_map[i,j,l])
    end do
  end do
end do
```



Advanced model MX

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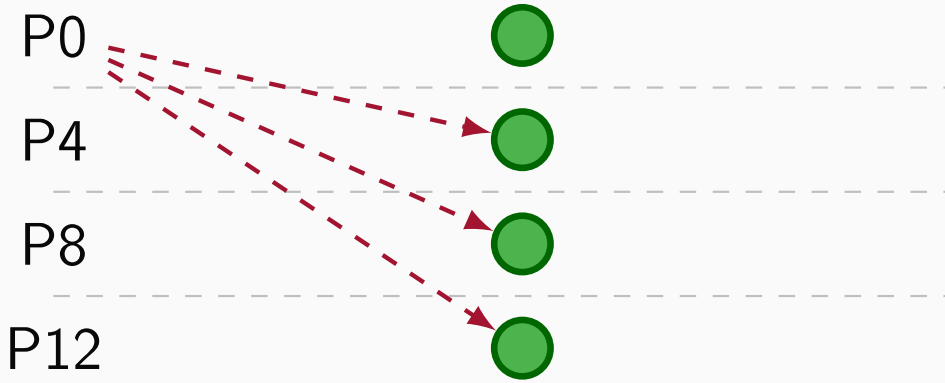
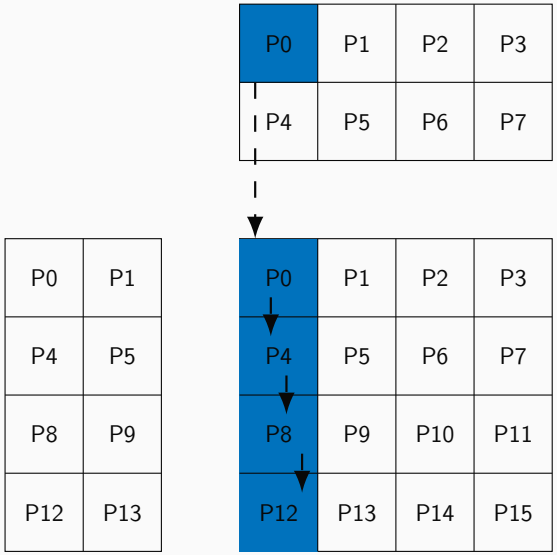
- MX-1 Explicit task mapping
- MO-2 Comms. inferred
- MX-3 Implicit reduction pattern



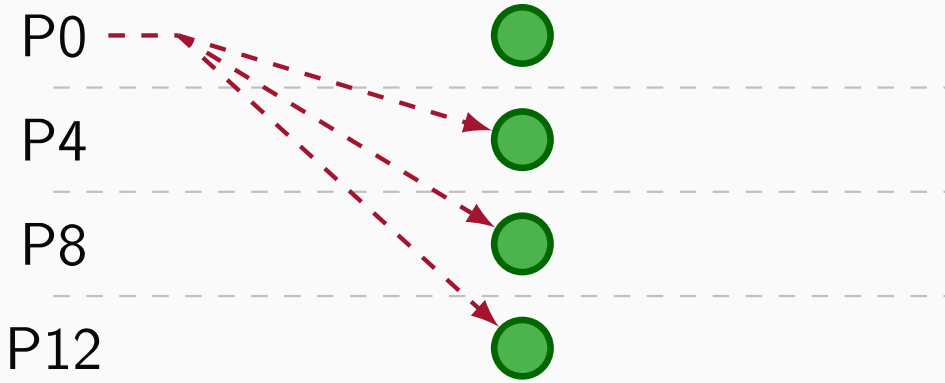
Key 3 – Communications

```
!data_map: A,B,C distributed on one
     layer
!task_map: executing node of A_{i,l}B_{l,j}
!dyn_tree: type of broadcast tree
call bind_methods(C, init, sum)
do i=1,m
  do j=1,n
    do l=1,k
      call insert_task(gemm,
                       A_{i,l}:R,
                       B_{l,j}:R,
                       C_{i,j}:RANK_REDUX,
                       task_map[i,j,l])
    end do
  end do
end do
```



Advanced model MX

- MO-0 Data mapping
- MX-1 Explicit task mapping
- MX-2 **Coll. comms.** inferred [1]
- MX-3 Implicit reduction pattern



[1] Denis, Jeannot, Swartvagher, and Thibault, 2020.

Ideal expression

```
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call bind_methods(C, init, sum)
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    end do
  end do
end do
```

- `task_map` can be set to cover any SUMMA variant
- Agnostic of:
  - the data distribution
  - the scheduling
  - the processing units

Advanced model `MX`

- `M0-0` Data mapping
- `MX-1` **Explicit** task mapping
- `MX-2` **Collective** communications **inferred** from task mapping
- `MX-3` **Implicit** reduction pattern

Ideal expression - task mappings

- 2D-C-Stat owner of C computes
  - `task_map[i,j,l]` $= j \,\%\, c + c * (i \,\%\, r)$
  - `access_mode` $=$ `RW`

- 2D-A-Stat owners of A compute
  - `task_map[i,j,l]` $= l \,\%\, c + c * (i \,\%\, r)$
  - `access_mode` $=$ `RANK_REDUX`

- 2.5D-C-Stat several nodes compute
  - `task_map[i,j,l]` $= j \,\%\, c + c * (i \,\%\, r) + rc \frac{l}{k/h}$
  - `access_mode` $=$ `RANK_REDUX`

The advanced model allows to **cover all variants** of SUMMA algorithms with three nested loops.
In a **distribution-agnostic** fashion.

Ideal expression - task mappings

- 2D-C-Stat owner of C computes
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  - `task_map[i,j,l]` $= l \,\%\, c + c * (i \,\%\, r)$
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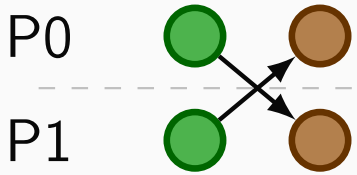

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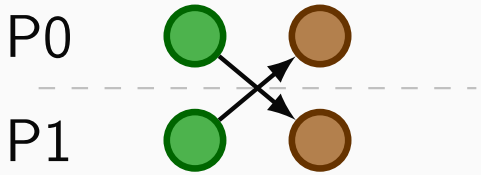

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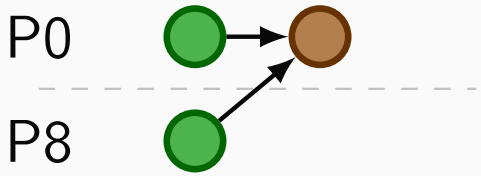

The advanced model allows to **cover all variants** of SUMMA algorithms with three nested loops.
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Ideal expression - task mappings

- 2D-C-Stat owner of C computes
  - `task_map[i,j,l]` $= C_{i,j}.owner\_rank$
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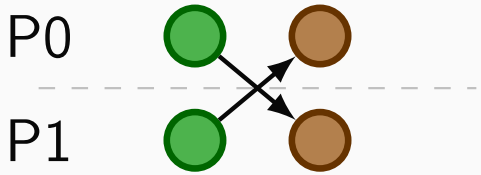

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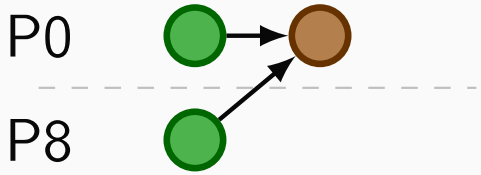

The advanced model allows to **cover all variants** of SUMMA algorithms with three nested loops.
In a **distribution-agnostic** fashion.

EXPERIMENTAL RESULTS

Experimental setup

- **Hardware**: Très Grand Centre de Calcul (TGCC)
  - **Irène - Skylake**
    - Dual-processor Intel Skylake 8168 @ 2.7 GHz
    - 24 cores per processor, 192 GB DDR4 memory
    - Infiniband EDR, 4x links, «fat tree» topology
  - **Irène - Rome**
    - Dual-processor AMD Rome (Epyc) @ 2.6 GHz
    - 64 cores per processor, 256 GB DDR4 memory
    - Infiniband HDR100, 2x links, «dragonfly» topology

Experimental setup

- **Software**: GNU 9.3.0, MKL 21.3.0
  - `qr_mumps` **ours** – newMadeleine, 1 MPI / node
    - StarPU with advanced model `MX` + seq. BLAS
    - 2.5D A,B,C-stationary version
  - `scalapack` – OpenMPI 4.0.5, 2 cores / MPI
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  - `chameleon` – newMadeleine, 1 MPI / node
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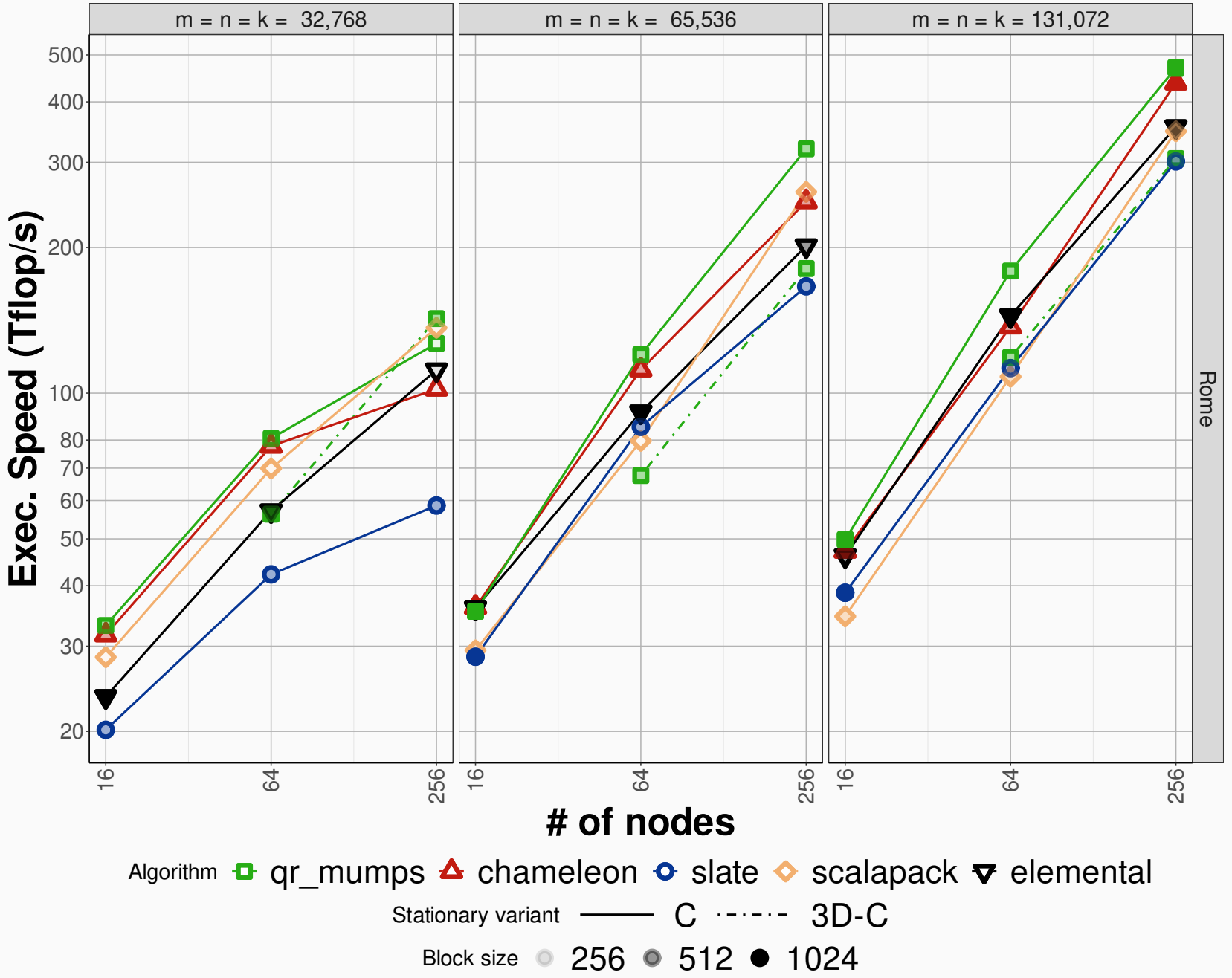
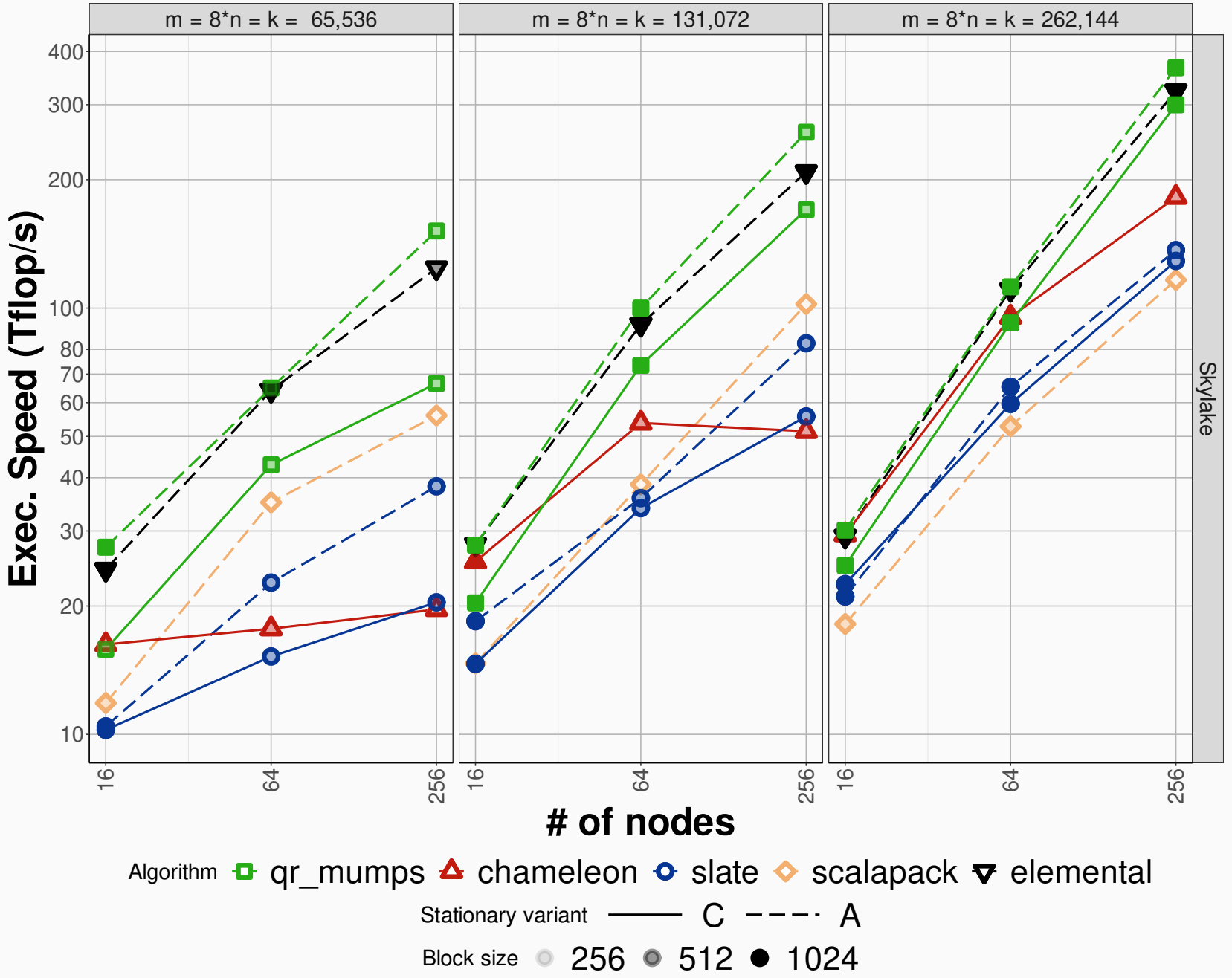
Rome (up to 32,768 cores) – square matrices, DGEMM



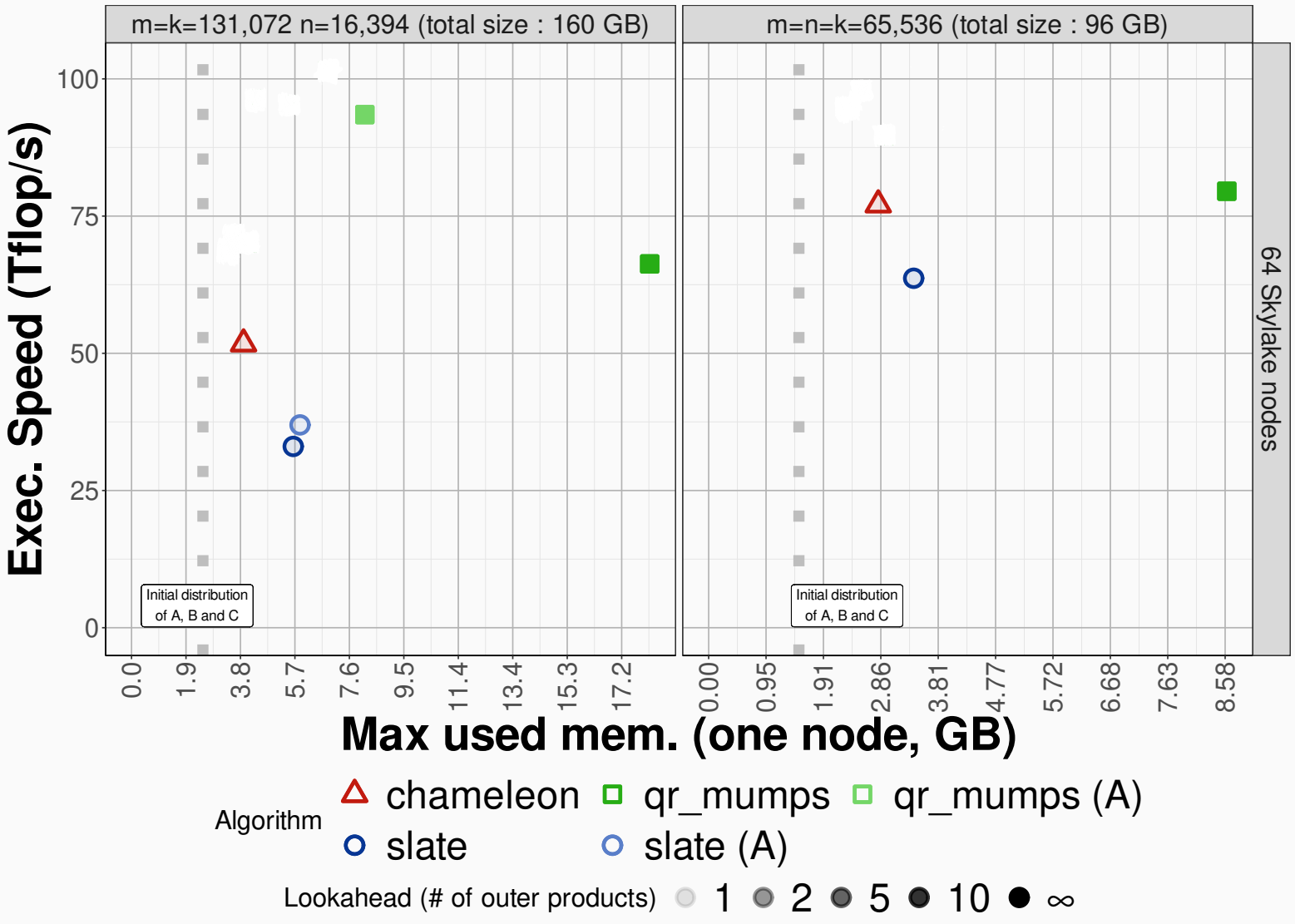
Skylake (up to 12,288 cores) – large A, DGEMM



Skylake – memory consumption

Submitting the **full DAG** allows **greedy** memory consumption

Task window mechanisms can help limit memory consumption



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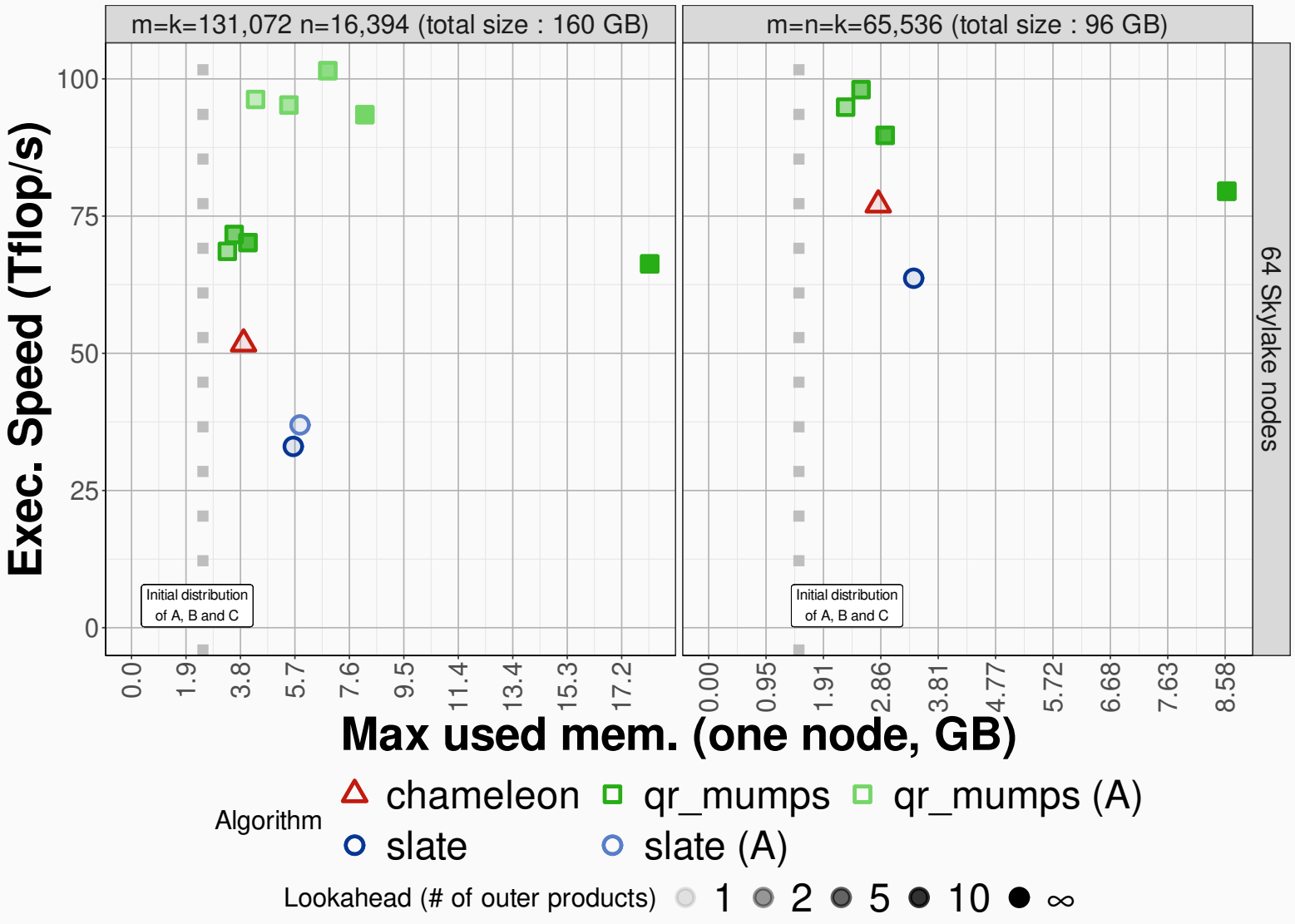


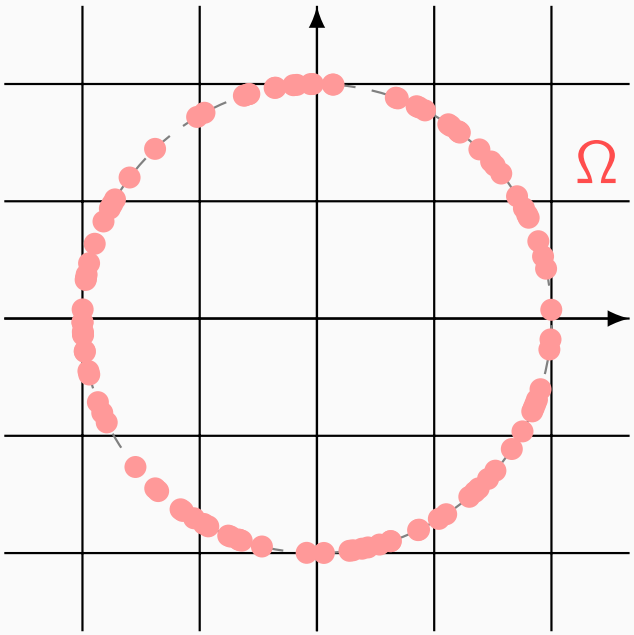
APPLICATION TO MACHINE LEARNING

Random linear algebra – background

Unsupervised learning:
We search for **eigencouples** of A, $n \times n$ matrix.

Two *limitations*:

- SVD is very costly $\sim O(n^3)$
- SVD is complex to parallelize



$A \times \Omega \sim O(n^2 k)$ if Ω is $n \times k$.

$\Rightarrow$ Approximating eigenvectors is *relatively cheap*.

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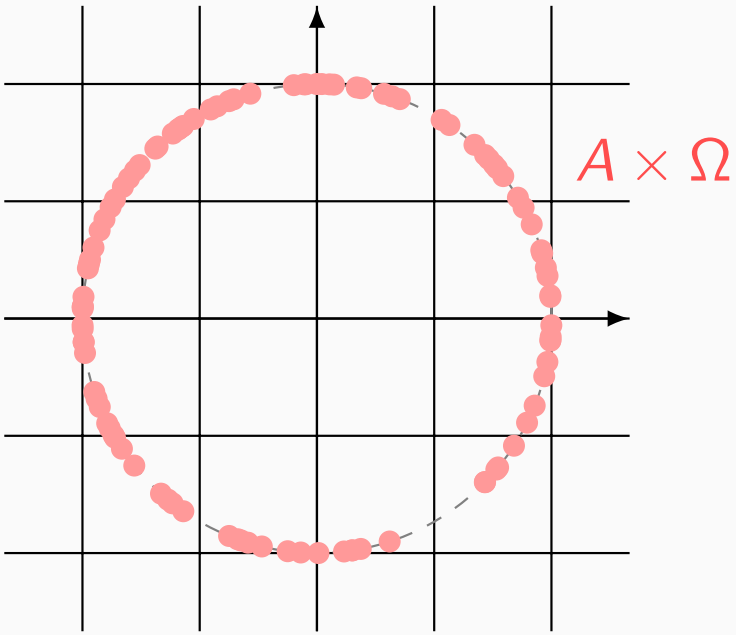

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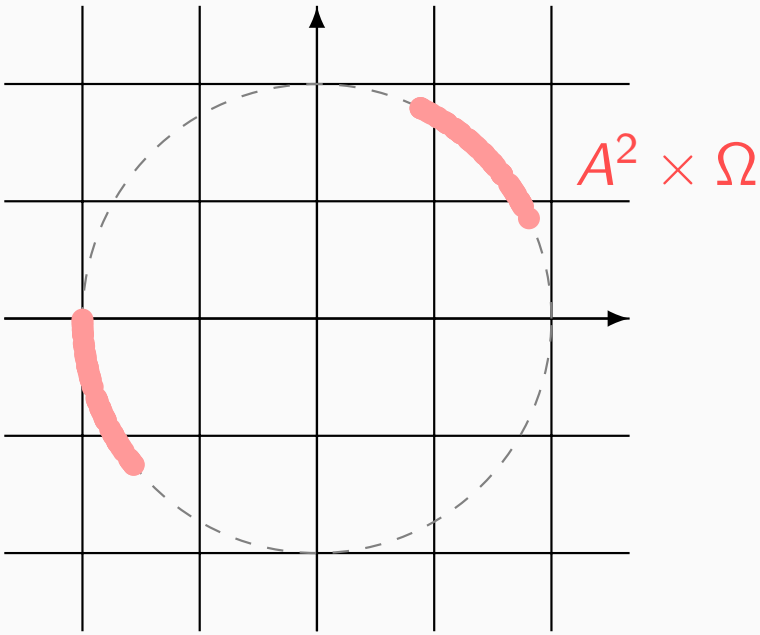

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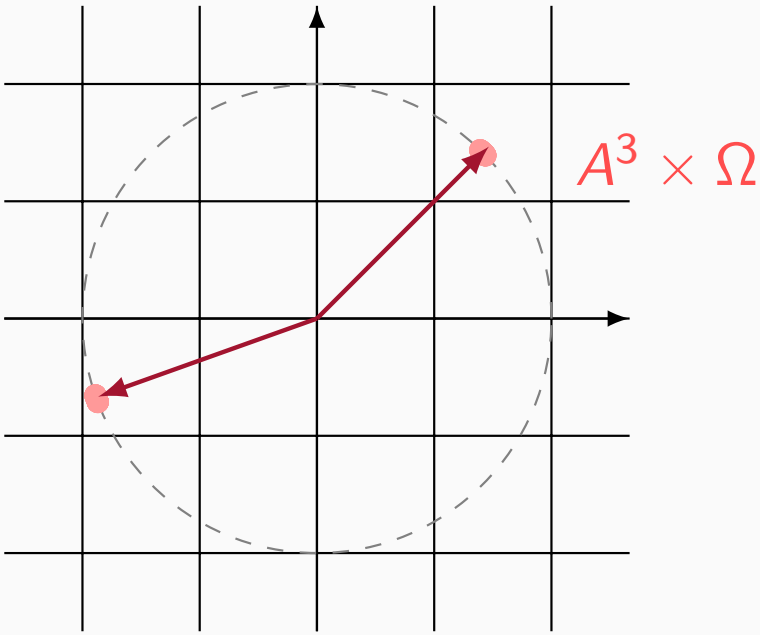

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Randomized SVD algorithm

```
D <- random_sample(n)
G <- gramian_matrix(D)
Ω <- random_matrix(n,k)
A <- GΩ
Q, R <- qr(A)
Y <- Q^T G
U, Σ, V <- svd(Y)
```

Some properties

G is a symmetric matrix.

The most costly operations are

- $G\Omega \sim O(n^2 k)$
- $Q^T G \sim O(n^2 k)$

Tradeoffs between `GEMM` and `SYMM`:

- `SYMM` communicates twice more than `GEMM`
  - A given column of G is stored over $p + q$ nodes instead of p with 2DBC.
- `GEMM` consumes twice more memory than `SYMM`
  - The whole matrix G is allocated.

Unless ...

- New distributions are discovered (they have been!)
- Our programming model adapts to any distributions (it does !)

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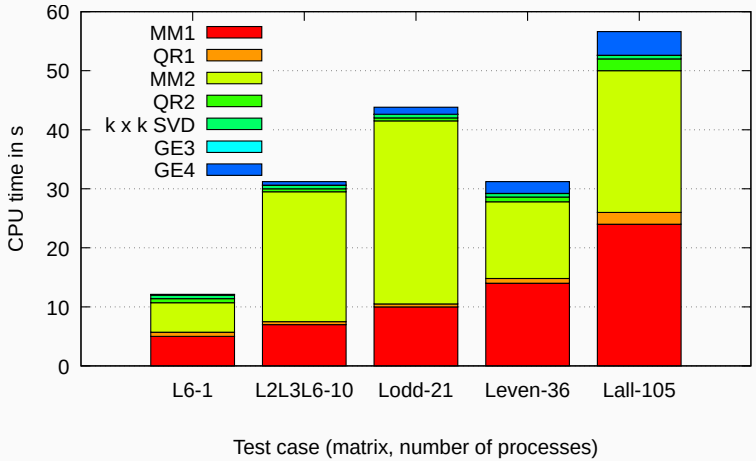
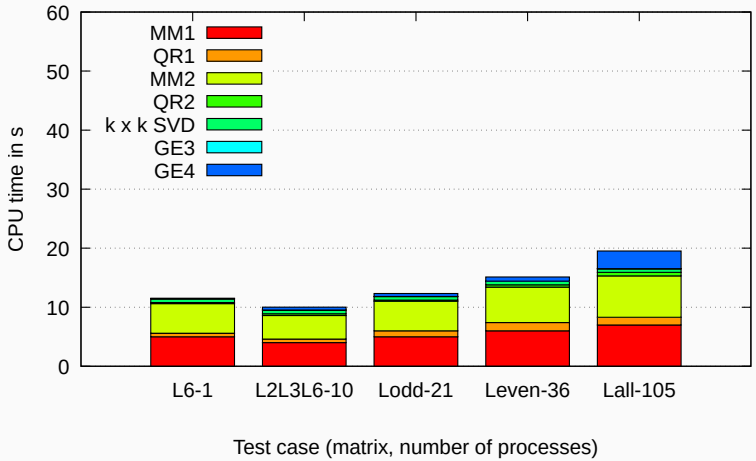
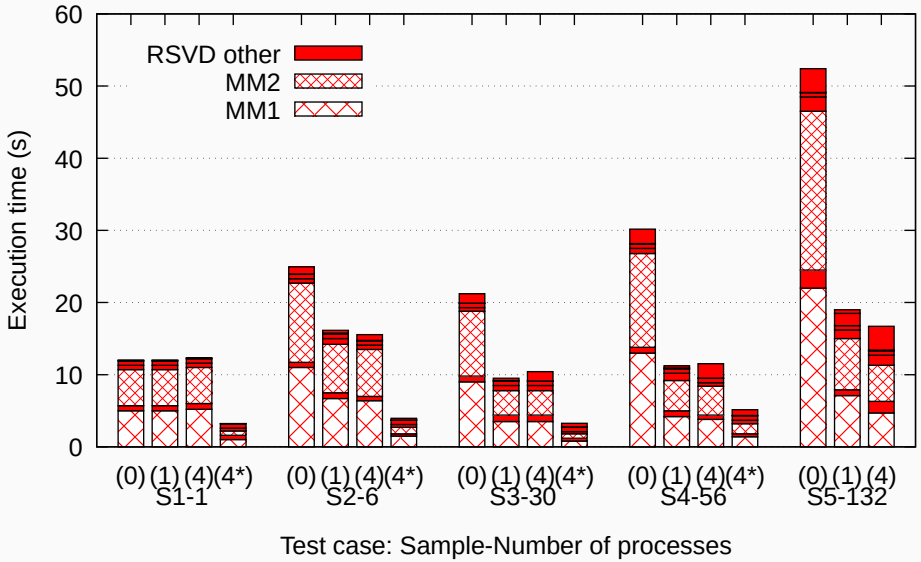
Random linear algebra – experiments



Legacy algorithm



A-stationary SYMM



- (0) Legacy algorithm
- (1) A-stationary GEMM
- (4) A-stationary SYMM
- (4*) A-stationary SYMM + GPU

CONCLUSIONS

Contributions

- Show **the STF programming model** can be suitably **extended** to **express** a complex distributed-memory algorithm
  - **Portable**, easily **maintainable**
  - Independant of matrices' distribution, workflow's scheduling
  - **Competitive** with reference libraries

Technical report: `https://hal.inria.fr/hal-03588491/`

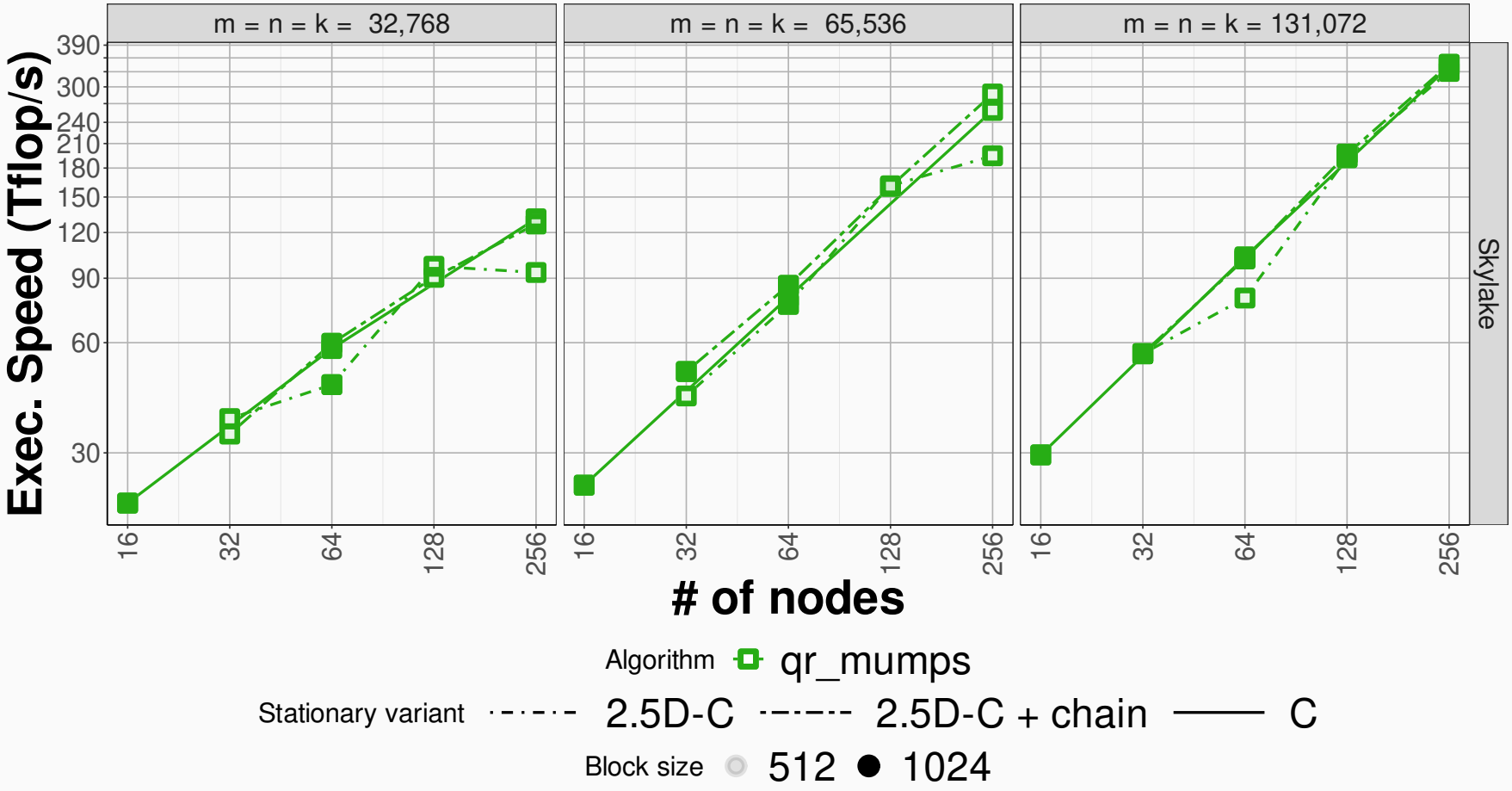
On-going work

- Implementing factorizations algorithms
  - How to replicate tasks ? How to setup alternative sources for a block ?
- Studying the scheduling of communication patterns in GEMM
  - In collaboration with O. Beaumont, A. Denis, L. Eyraud-Dubois, E. Jeannot, M. Vérité, P. Swartvagher

ON-GOING WORK

Extensive study on communication ordering for GEMM

Experiments questionning the scheduling of communications



⇒ In collaboration with:

Olivier Beaumont, Alexandre Denis, Lionel Eyraud-Dubois, Emmanuel Jeannot, Mathieu Vérité, Philippe Swartvagher

Dense Factorizations (LU, Cholesky)

2.5D factorization algorithms have **more complex** critical path.

They require more advanced key functionalities:

1. Accumulation and reduction of **updates over layers**
2. **Replication** of factorization tasks
3. **All-reduce pattern** to implement tournament pivoting

The programming model currently lacks support for 2. and 3.

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BACKUP SLIDES

Practical expression

Some common operations are done before switching on the `stat` parameter:

- Binding C to the `init` and `sum` codelets
- (submitting) the scaling of C by β

2.5D-A-Stat

```
do jh=1,n/h; do layer=1,h
  j = jh * layer
  do i=1,m
    do l=1,k
Ail => transa ? A_{l,i} : A_{i,l}
Blj => transb ? B_{j,l} : B_{l,j}
Cij => C_{i,j}
work_node = Ail%owner
          + r*c*layer
call insert_task( gemm,
  work_node:ON_NODE,
  Ail:R,Blj:R,
  Cij:RANK_REDUX )
    end do
    call mpi_redux_tree(C_{i,j})
  end do
end do; end do
```

2.5D-B-Stat

```
do ih=1,m/h; do layer=1,h
  i = ih * layer
  do j=1,n
    do l=1,k
Ail => transa ? A_{l,i} : A_{i,l}
Blj => transb ? B_{j,l} : B_{l,j}
Cij => C_{i,j}
work_node = Blj%owner
          + r*c*layer
call insert_task( gemm,
  work_node:ON_NODE,
  Ail:R,Blj:R,
  Cij:RANK_REDUX )
    end do
    call mpi_redux_tree(C_{i,j})
  end do
end do; end do
```

2.5D-C-Stat

```
do lh=1,k/h; do layer=1,h
  l = lh * layer
  do i=1,m
    do j=1,n
Ail => transa ? A_{l,i} : A_{i,l}
Blj => transb ? B_{j,l} : B_{l,j}
Cij => C_{i,j}
work_node = Cij%owner
          + r*c*layer
call insert_task( gemm,
  work_node:ON_NODE,
  Ail:R,Blj:R,
  Cij:RANK_REDUX )
    end do
  end do
end do; end do
do i=1,m; do j=1,n
  call mpi_redux_tree(C_{i,j})
end do; end do
```

StarPU – additional features ?

Some additional features to StarPU have been considered.

- Automatically insert reduction tasks
  - Further simplify factorization implementations

```
call starpu_mpi_redux(A_{I,I})
call insert_task(potrf, A_{I,I}:RW)
```

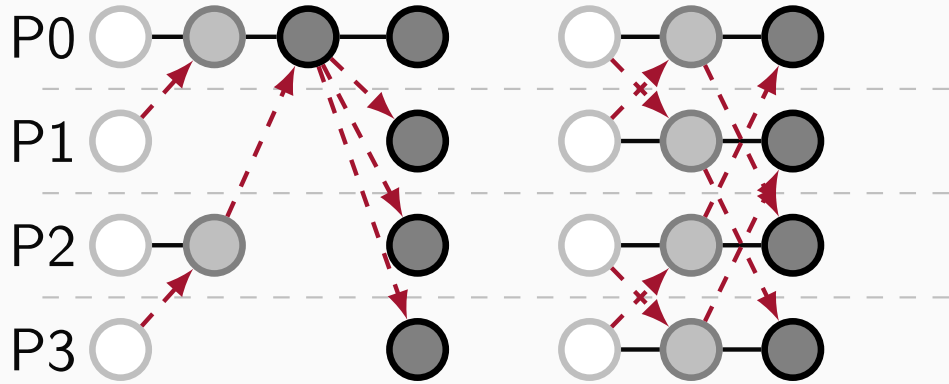
⇓

```
! implicit reduction
call insert_task(potrf, A_{I,I}:RW)
```

- Allow tasks replication across nodes
  - Required by state-of-the-art algorithms
  - Each resulting tile can be sent to different subsets of nodes

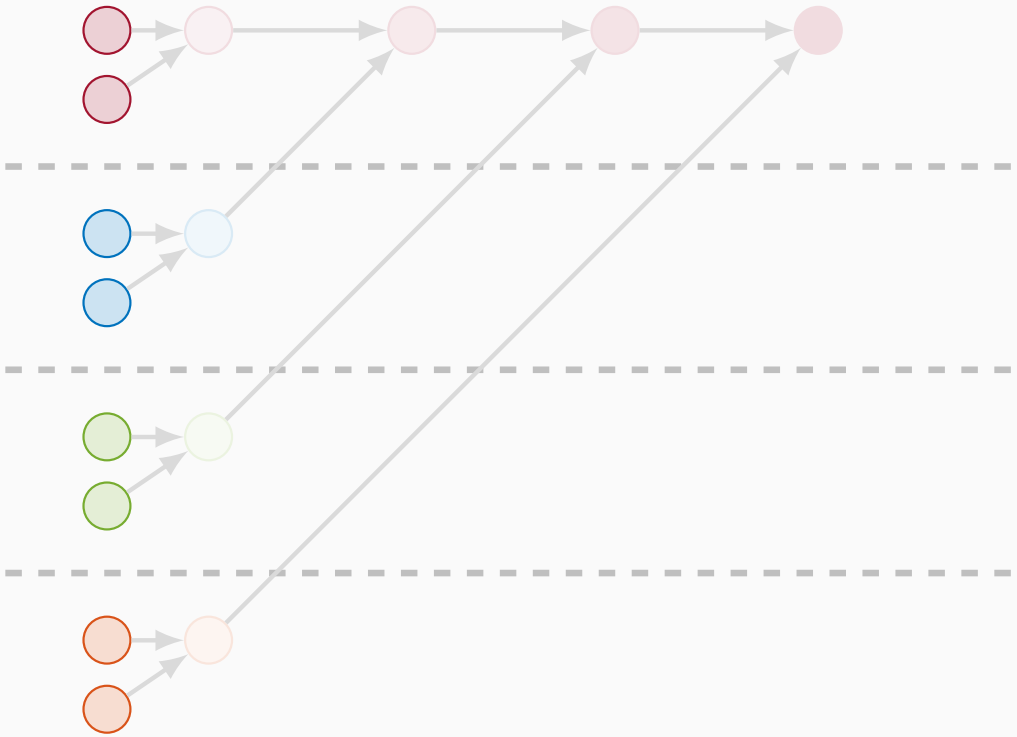
```
call insert_task(potrf, A_{I,I}:RW,
                 ON_NODES:task_map[I,I,:])
call insert_task(trsm, A_{I,I}:R, A_{i,I}:RW,
                 FROM_NODE:task_map[I,I,i%h])
```

- Allow all-reduce pattern
  - Shorten the critical path as replicated data is already available



Features of StarPU – 1.3

- `STARPU_REDUX`
  - One contribution per **core**
    - Intra-node reduction through binary tree
  - Remain available in StarPU (master)
- `starpu_mpi_redux_data`
  - **All** nodes in `MPI_COMM_World` contribute through a **flat** tree
  - **Blocking** method



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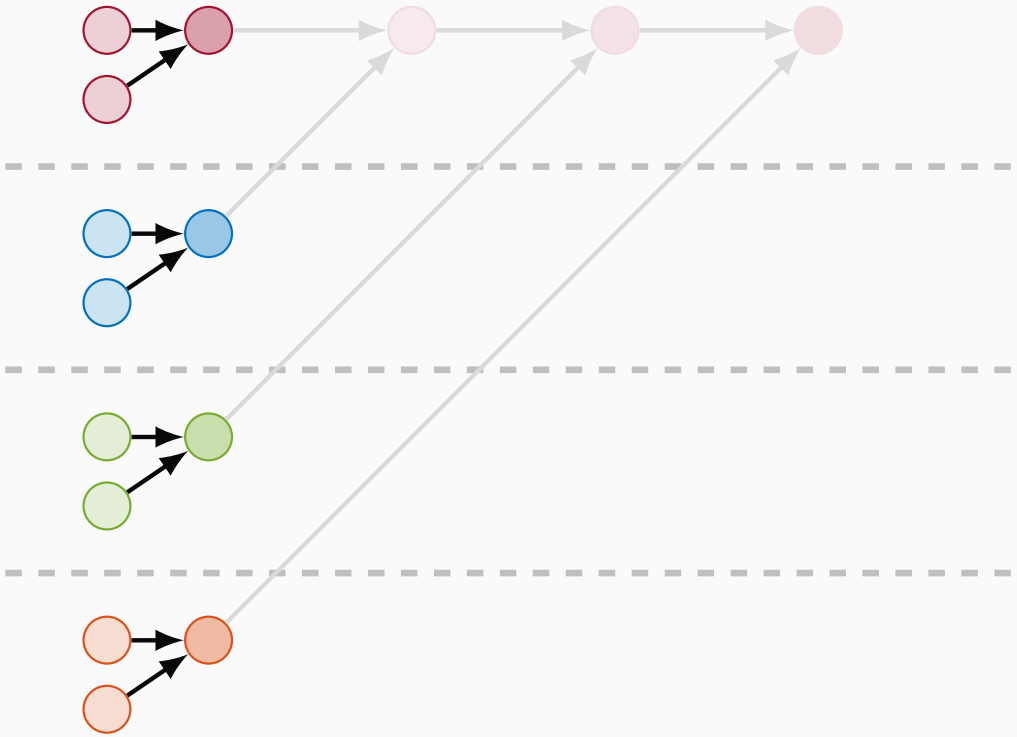

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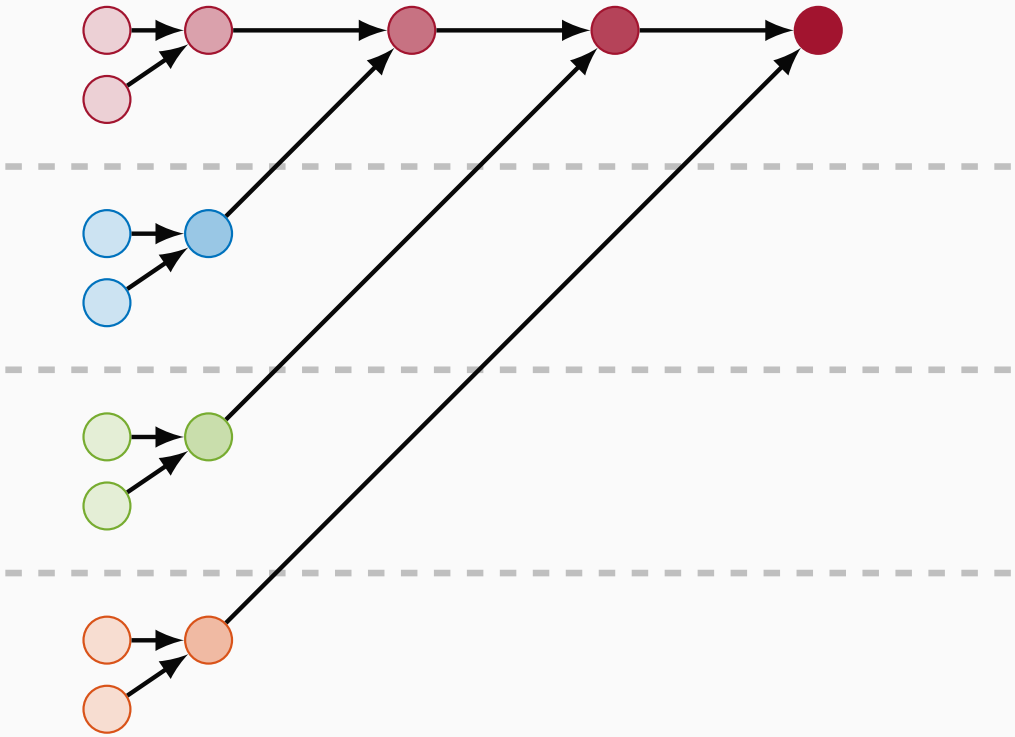
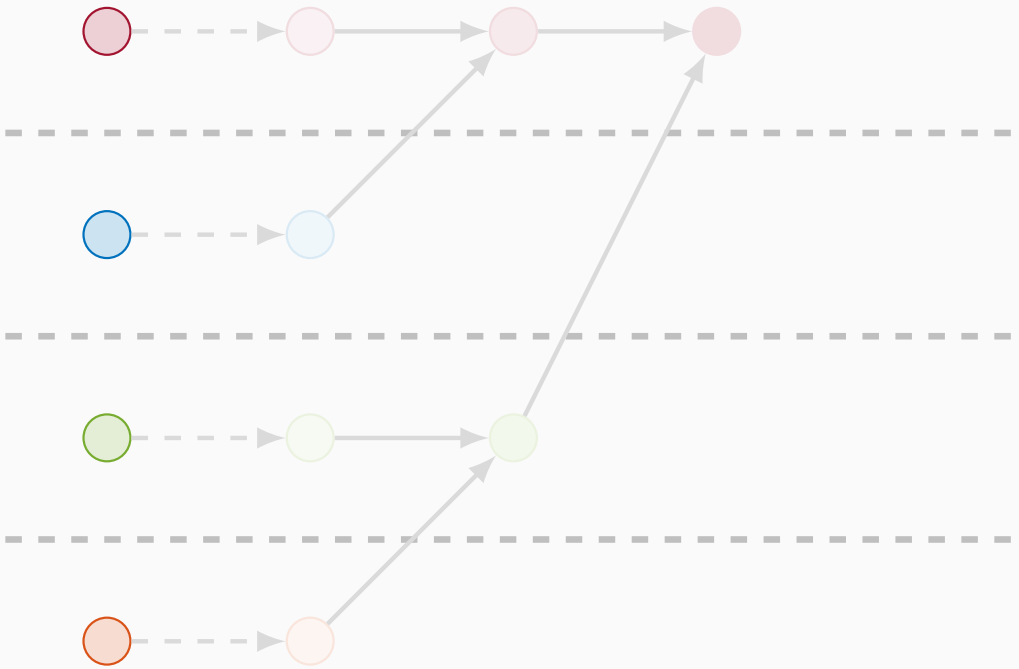


Features of StarPU – our contribution

- `STARPU_MPI_REDUX` (**Feature!** issue 3)
  - One contribution per **contributing node**
  - Interpreted as `STARPU_RW|STARPU_COMMUTE`
- `starpu_mpi_redux_data_tree` (**Enhancement!** merge req. 21)
  - All **contributing** nodes join in the reduction through a **n-ary** tree
  - **Non-blocking** method



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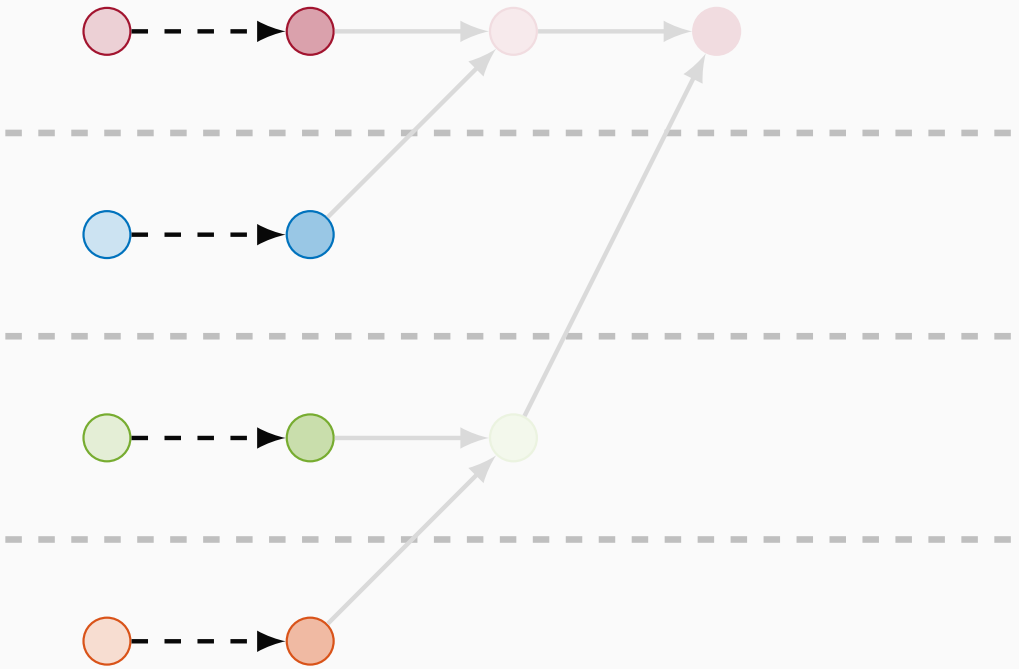

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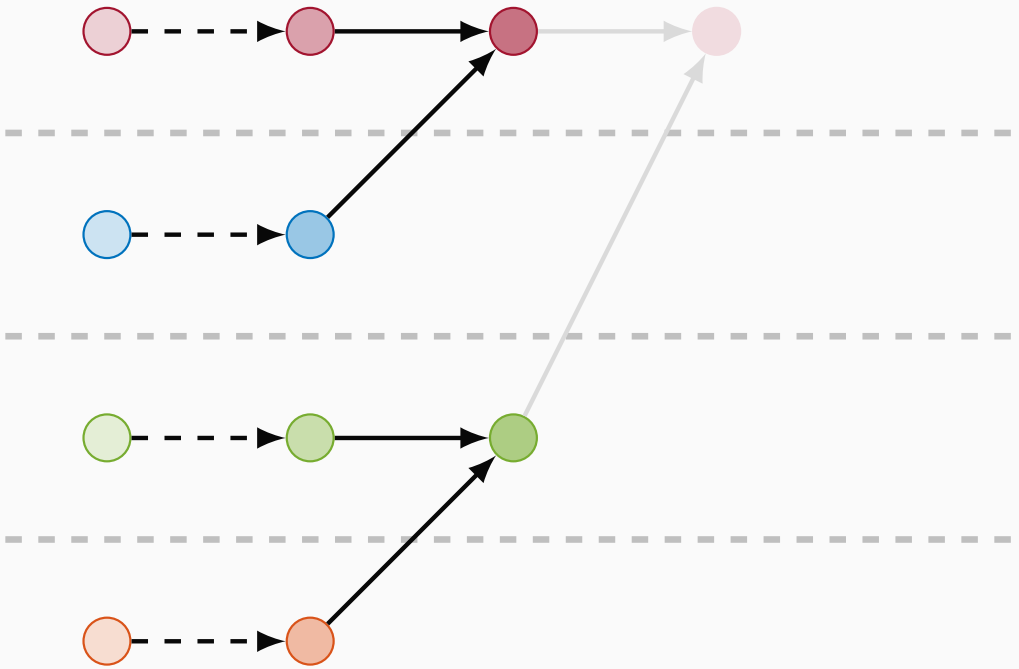

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