TASK-BASED PROGRAMMING MODELS FOR SCALABLE ALGORITHMS

Application to matrix multiplication

E. Agullo, A. Buttari, A. Guermouche, J. Herrmann, A. Jego

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INTRODUCTION

Algorithms, architectures and programming models

Architectures are becoming increasingly **large**, **heterogeneous** and **complex**. This has two effects:

- 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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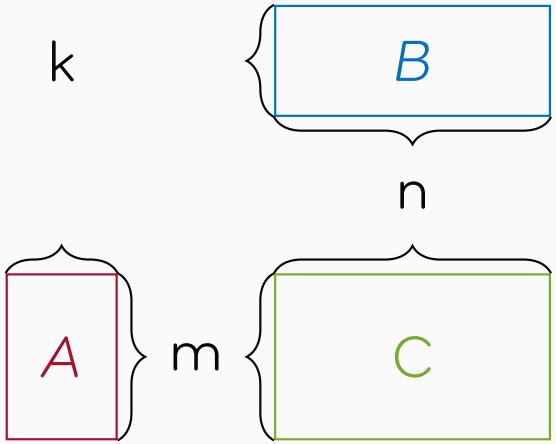
Algorithms, architectures and programming models

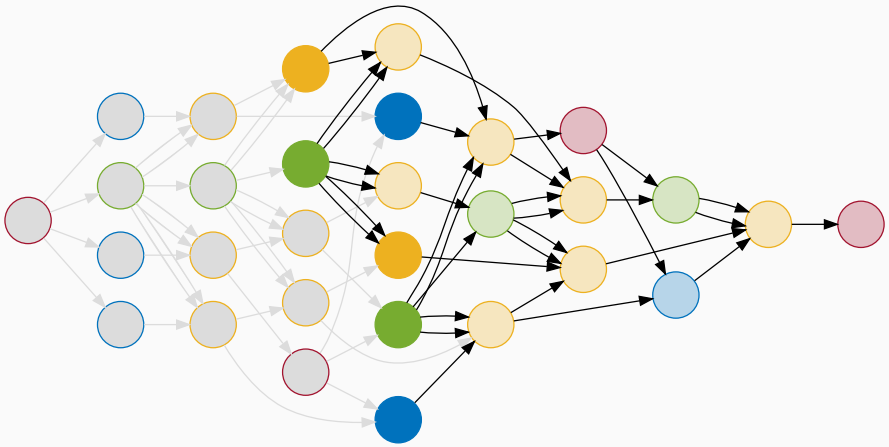
We take the following examples to answer this large question

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

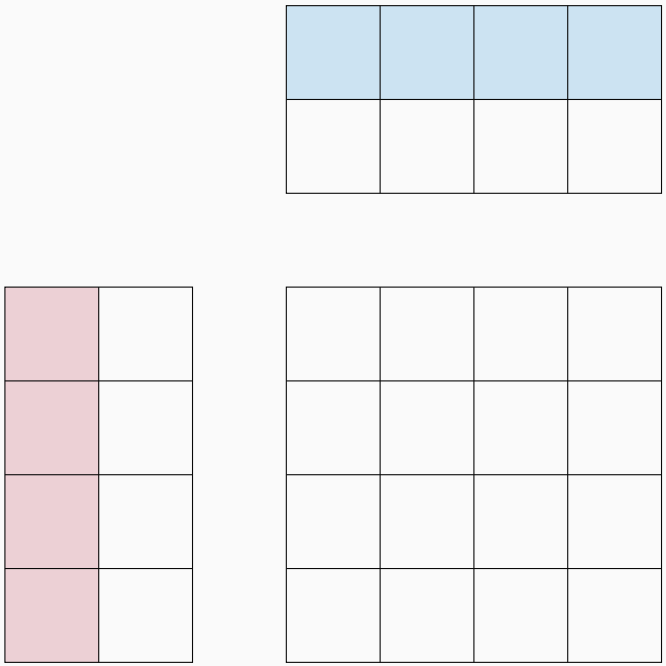
$$C = \alpha AB + \beta C$$



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



BACKGROUND



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

```
! I am r × c
do l=1, k
   forall i, i%p==r :
      bcast(A_{i,l}, r×*)
   forall j, j%q==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})
end do
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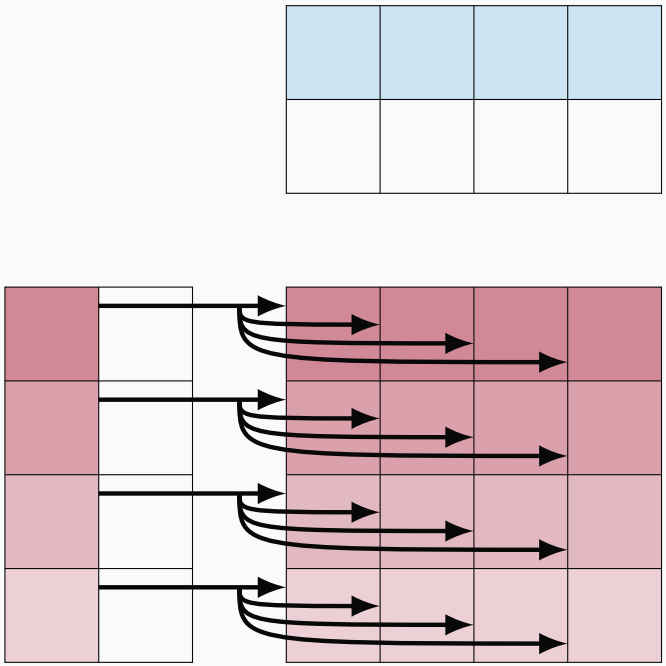
Geijn and Watts, 1997



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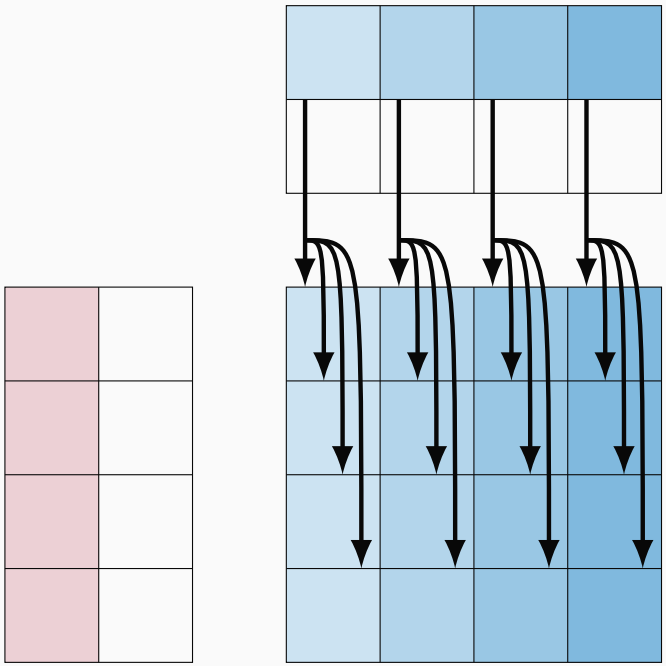

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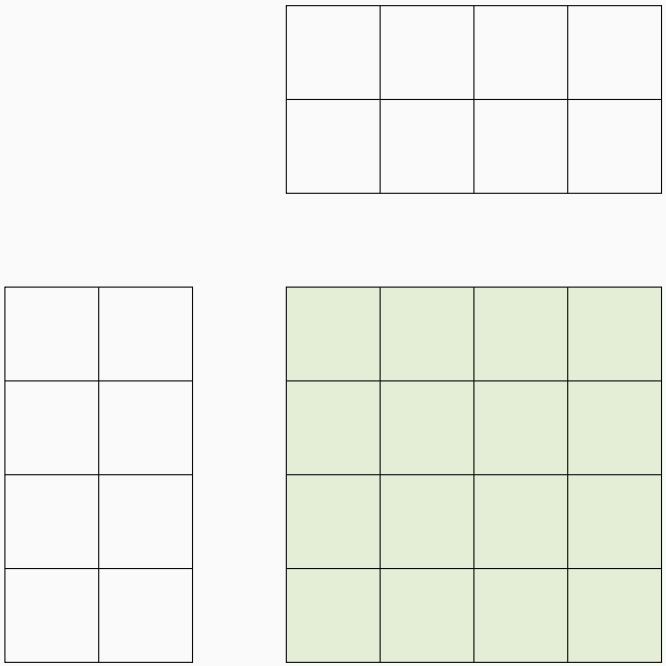

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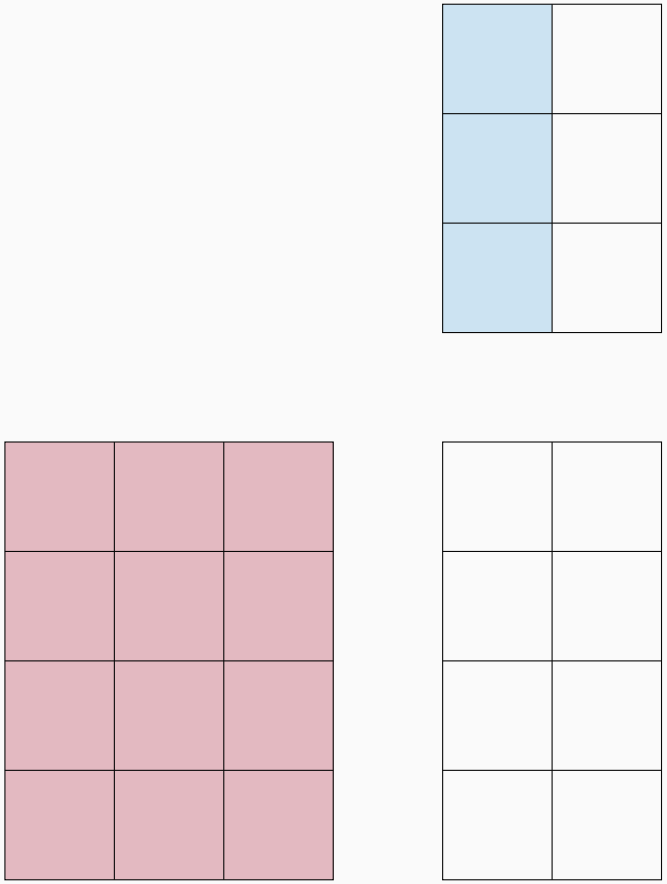

2D A-stationary SUMMA

- **Data mapping**
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  - column-wise scatter+broadcast of B
  - row-wise reduction of C

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do j=1, n
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      recv(B_{l,j}, l%p×j%q)
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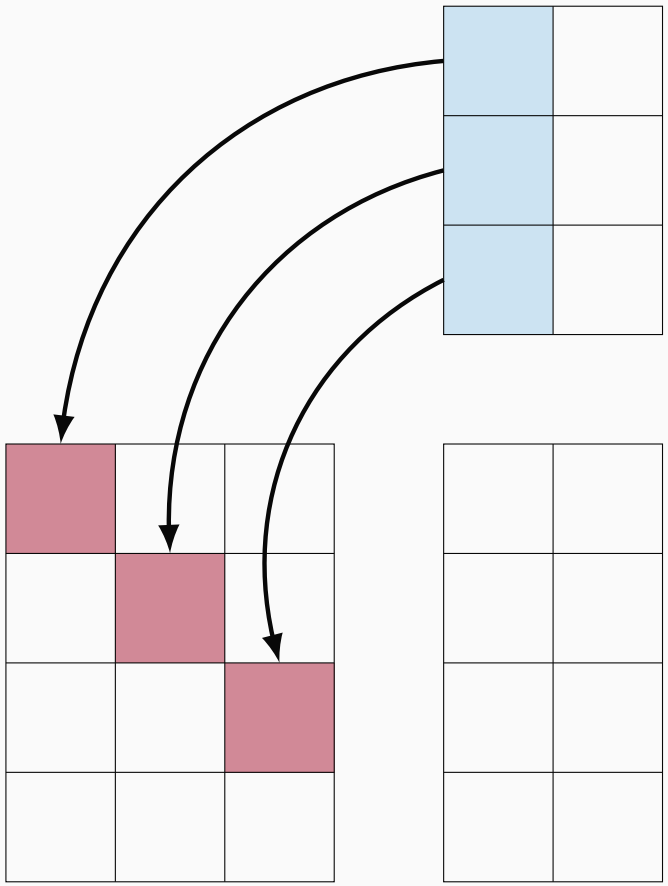

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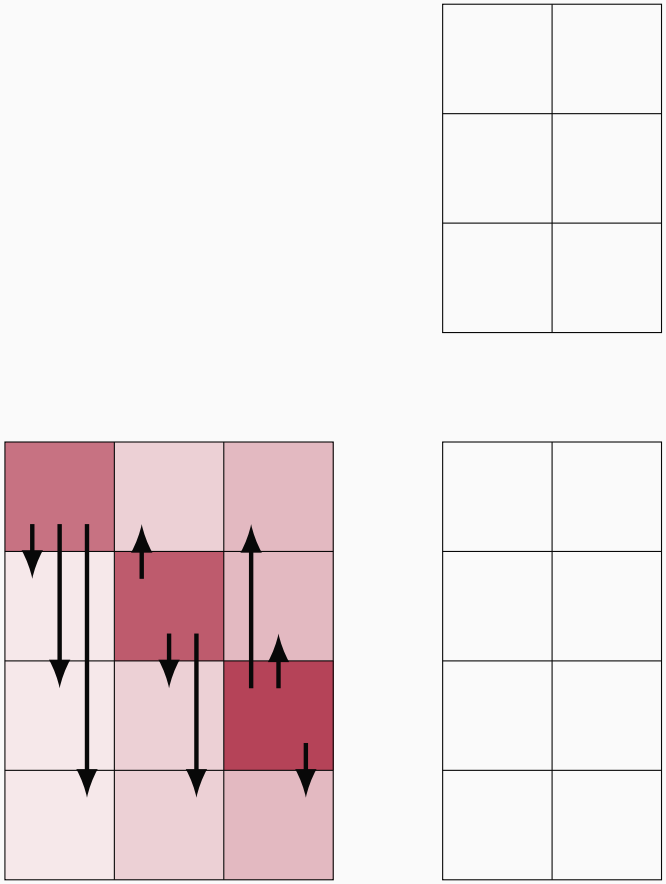

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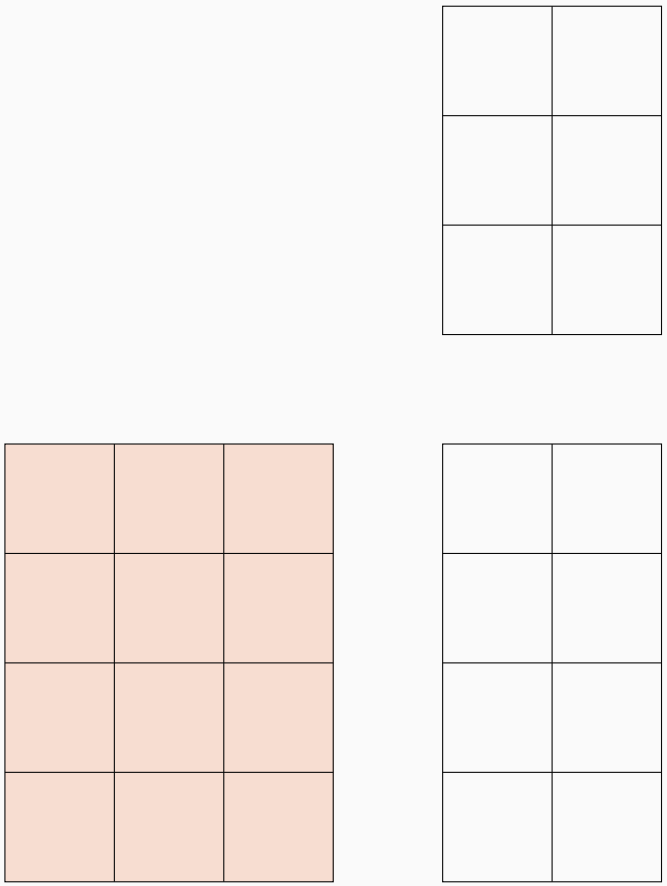

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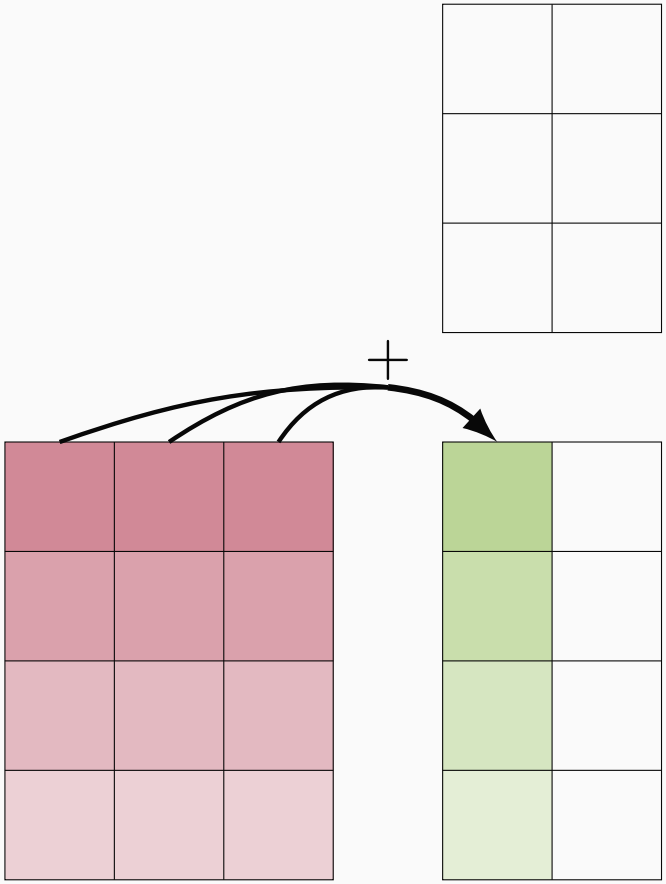

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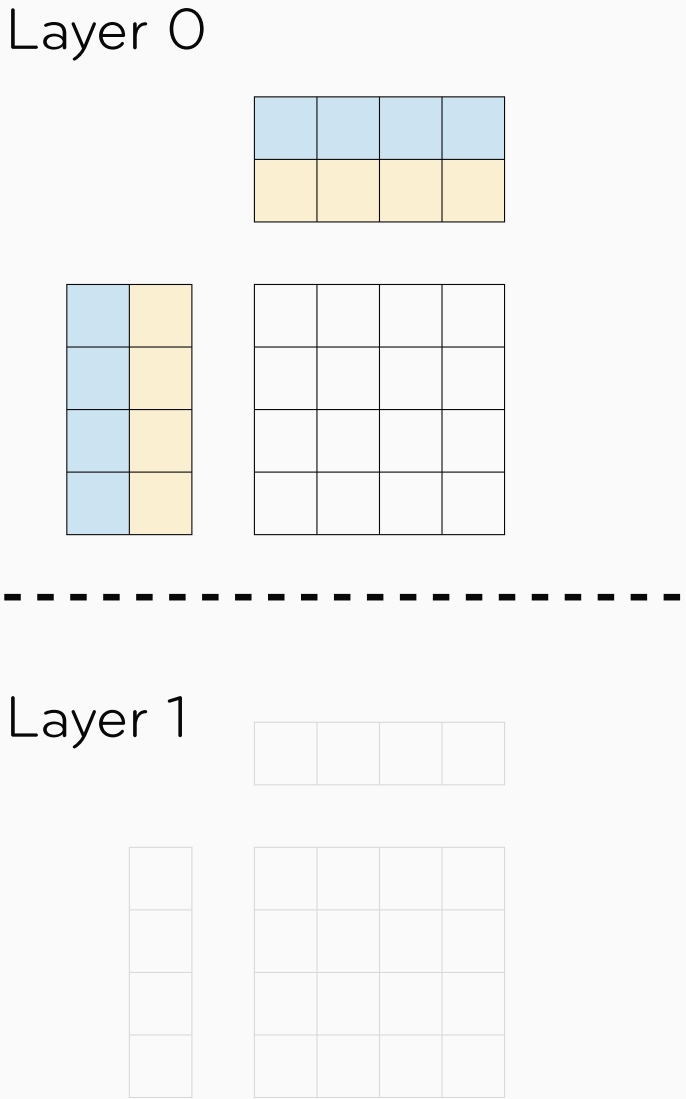

2.5D C-stationary SUMMA

- **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 :
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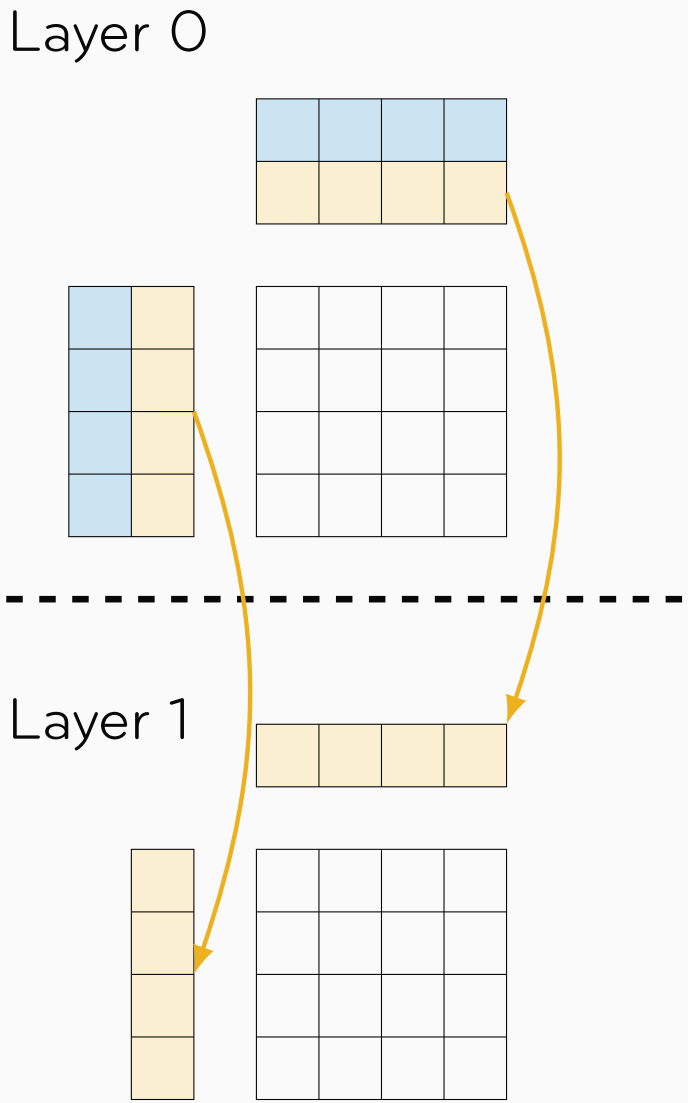
Irony, Toledo, and Tiskin, 2004



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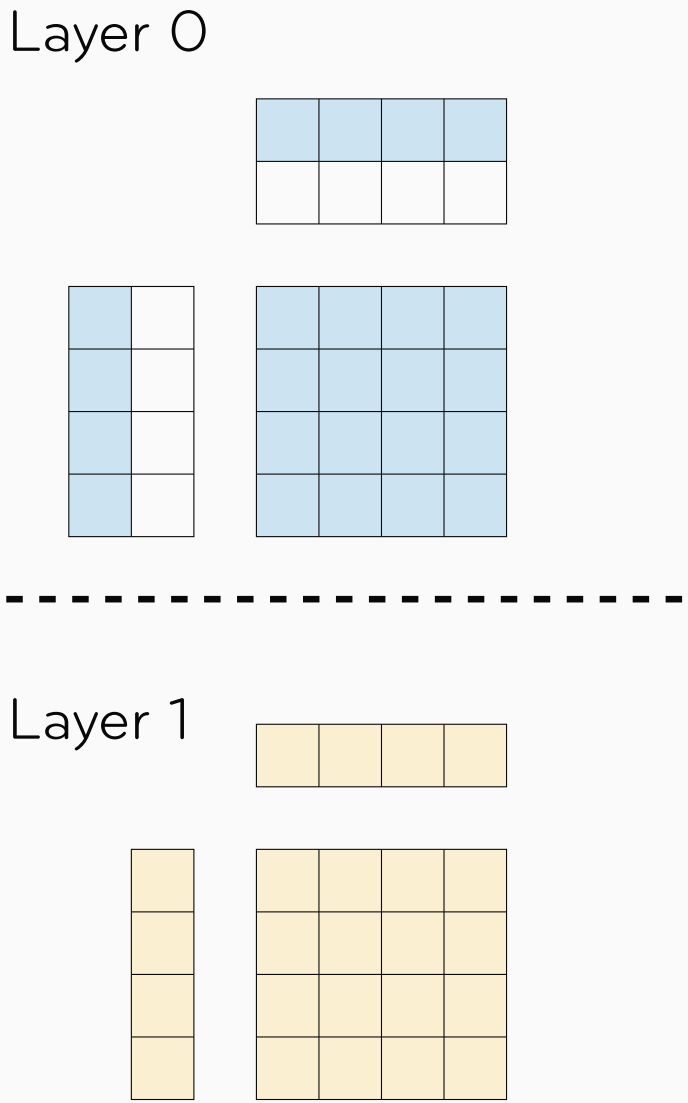

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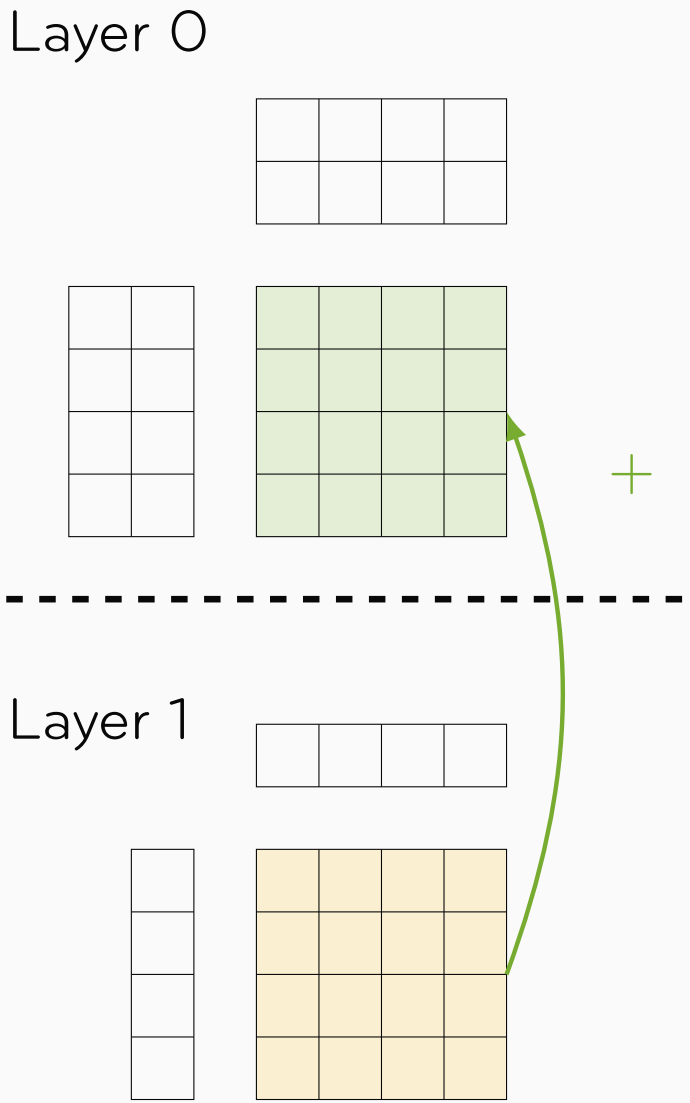

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The sequential task flow (STF) Model

Sequential GEMM

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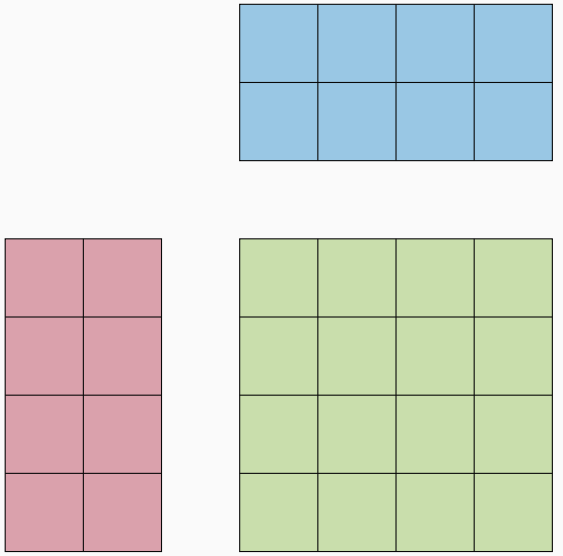

Shared-memory STF GEMM

```
do i=1,m
  do j=1,n
    do l=1,k
      call insert_task( gemm,
                    A(i,l):R,
                    B(l,j):R,
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DAG of GEMM

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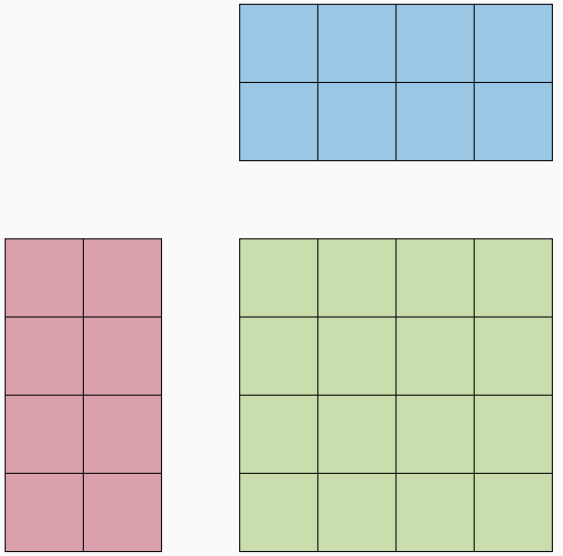

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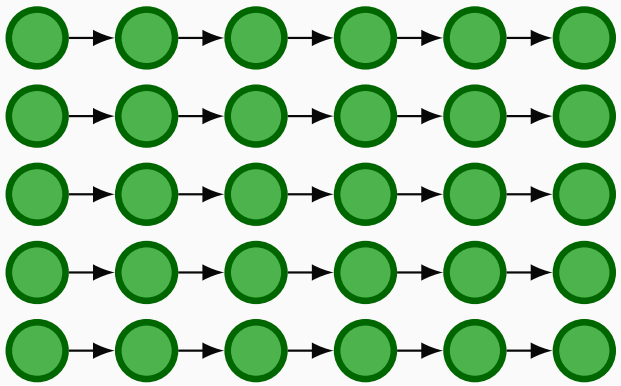

DAG of GEMM

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

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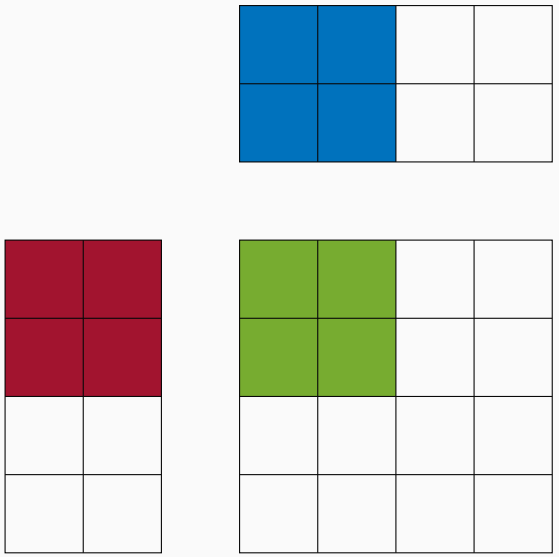
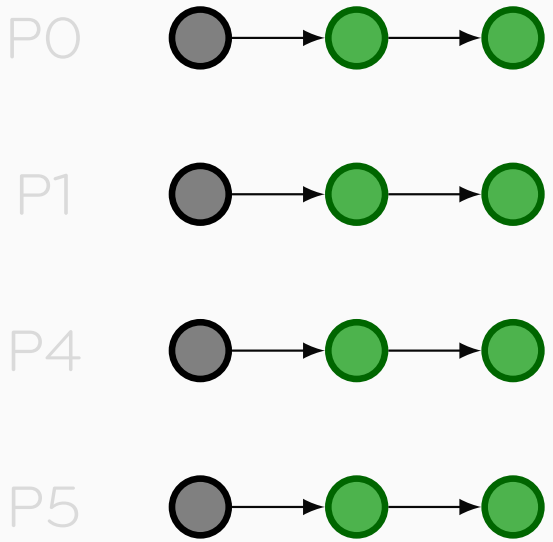


Baseline model (M0)[a]

- 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.

Baseline STF model

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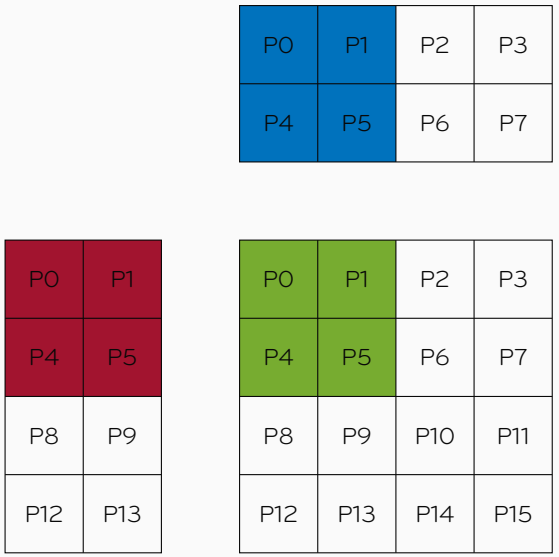

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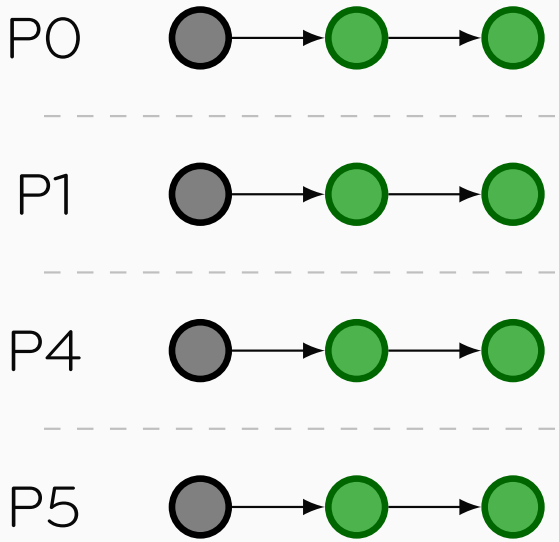

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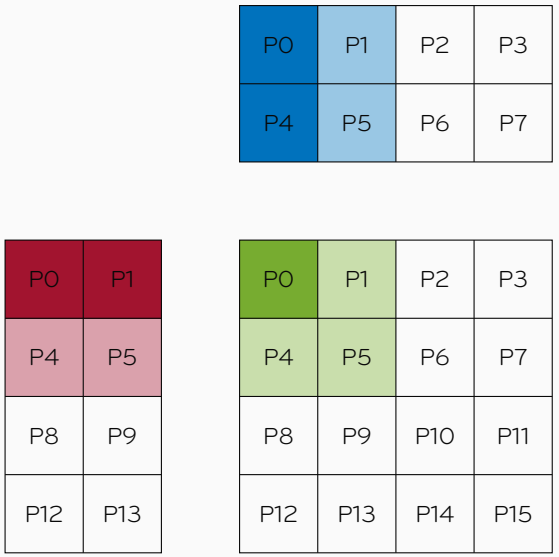

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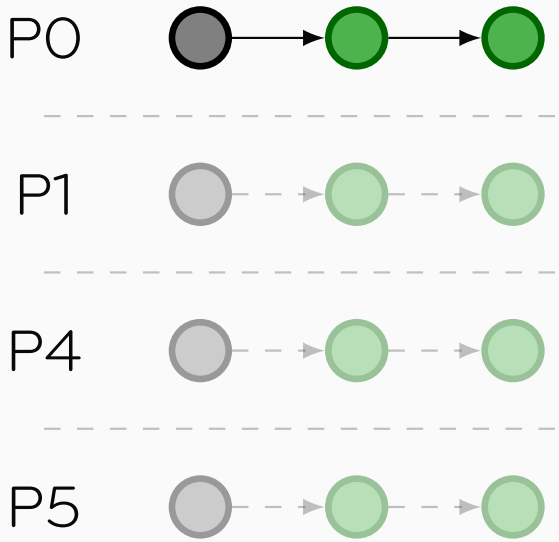

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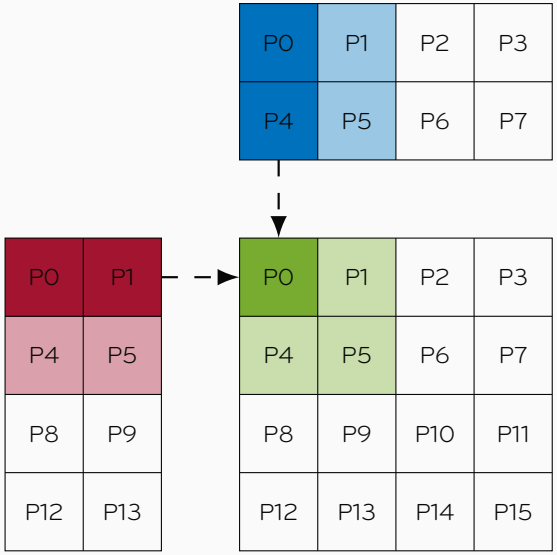

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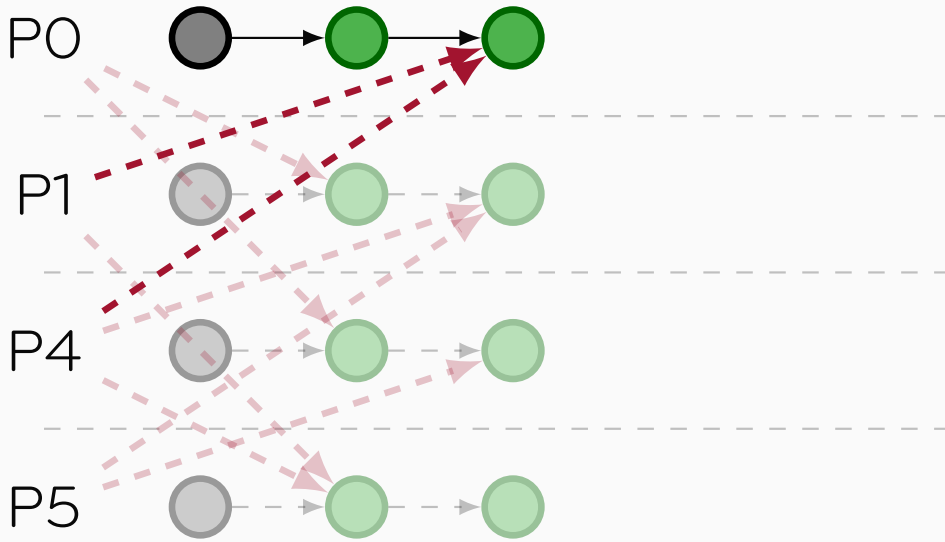
- M0-1 Task mapping **inferred** from DM (RW)
- M0-2 Point-to-point comms. **inferred** from TM



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

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.

Limits to the baseline model

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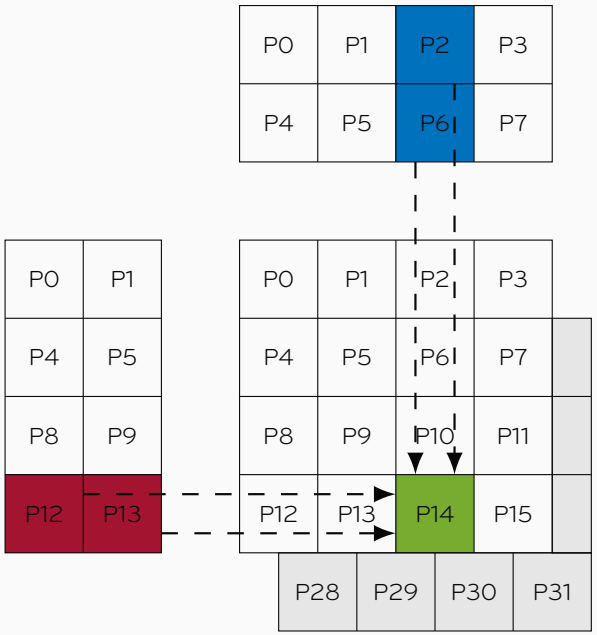
We have identified key functionalities required in a STF model `MX`, extended from `M0`, to allow the expression of SUMMA algorithms.

Key 1 – Task mapping

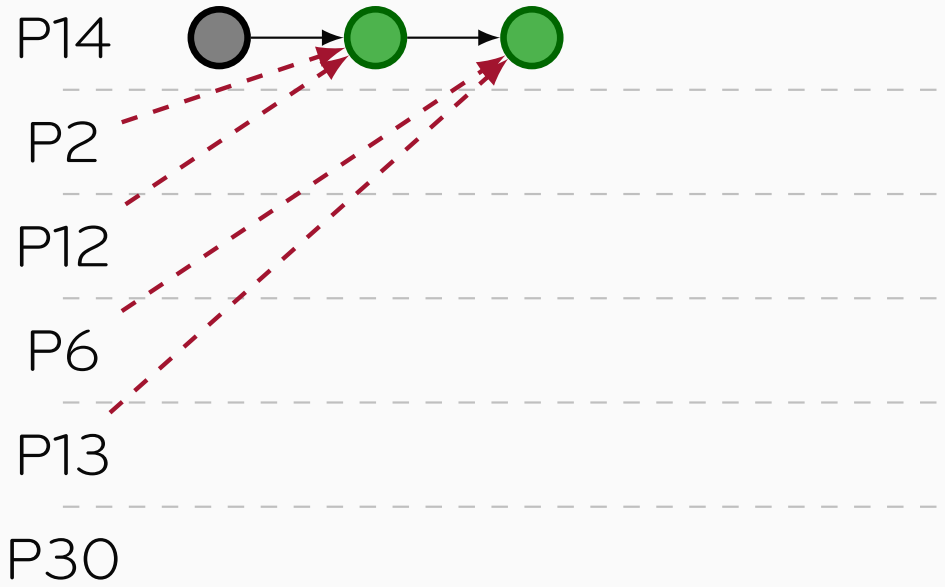
```
!data_map: A,B,C distributed on one layer
!
!

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



Advanced model MX

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



Key 1 – Task mapping

```
!data_map: A,B,C distributed on one layer
!task_map: executing node of A_{i,l}B_{l,j}
!

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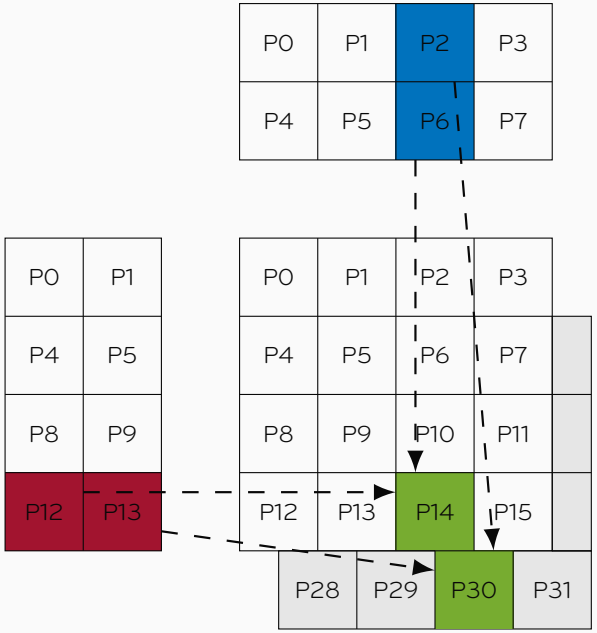
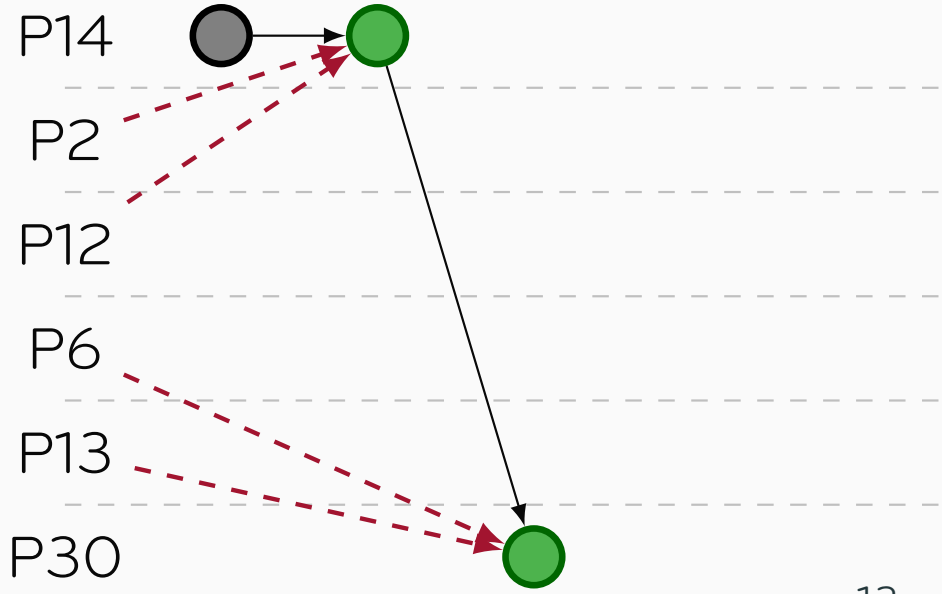
                       task_map[i,j,l])
    end do
  end do
end do
```



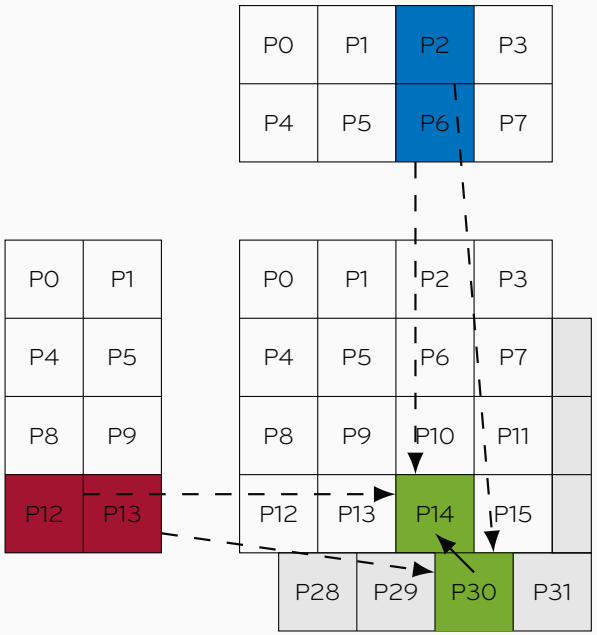
Advanced model MX

- M0-0 Data mapping
- MX-1 **Explicit** task mapping
- M0-2 Comms. inferred



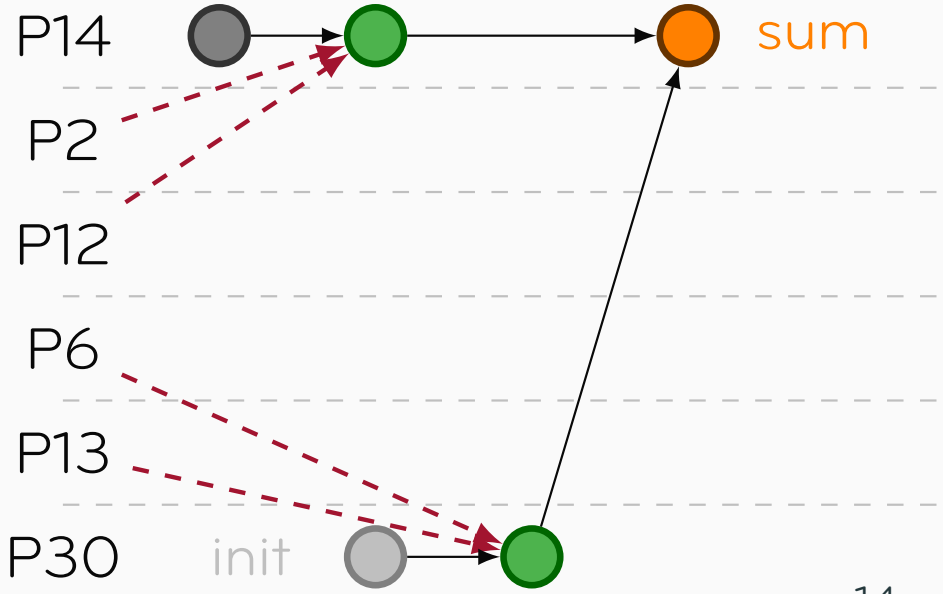
Key 2 – Reduction pattern

```
!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
end do
call reduce_to_initial_layer(C)
```



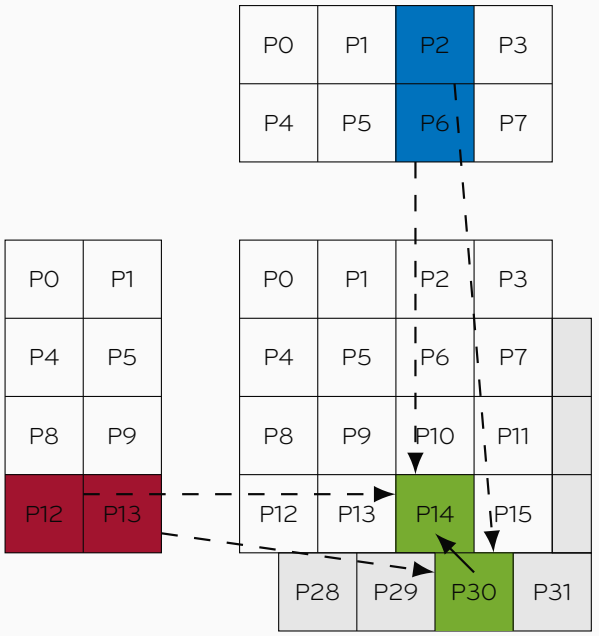
Advanced model MX

- 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 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}:RANK_REDUX,
                       task_map[i,j,l])
    end do
  end do
end do
call reduce_to_initial_layer(C)
```



Advanced model MX

- MO-0 Data mapping
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- MO-2 Comms. inferred
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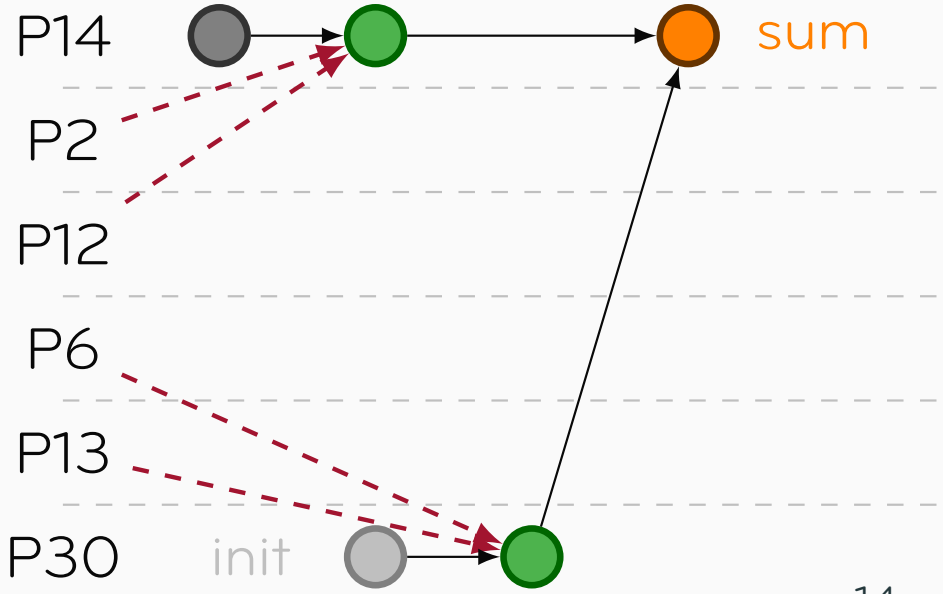

Key 2 – Reduction pattern

```
!data_map: A,B,C distributed on one layer
!task_map: executing node of A_{i,l}B_{l,j}
!
call 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,
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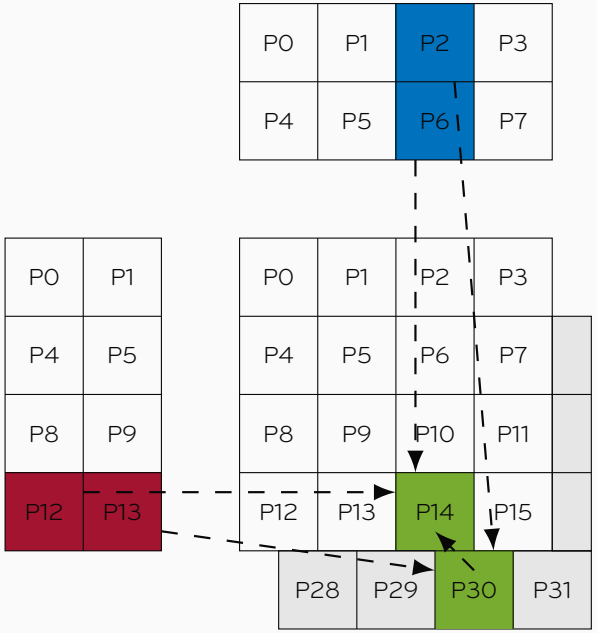
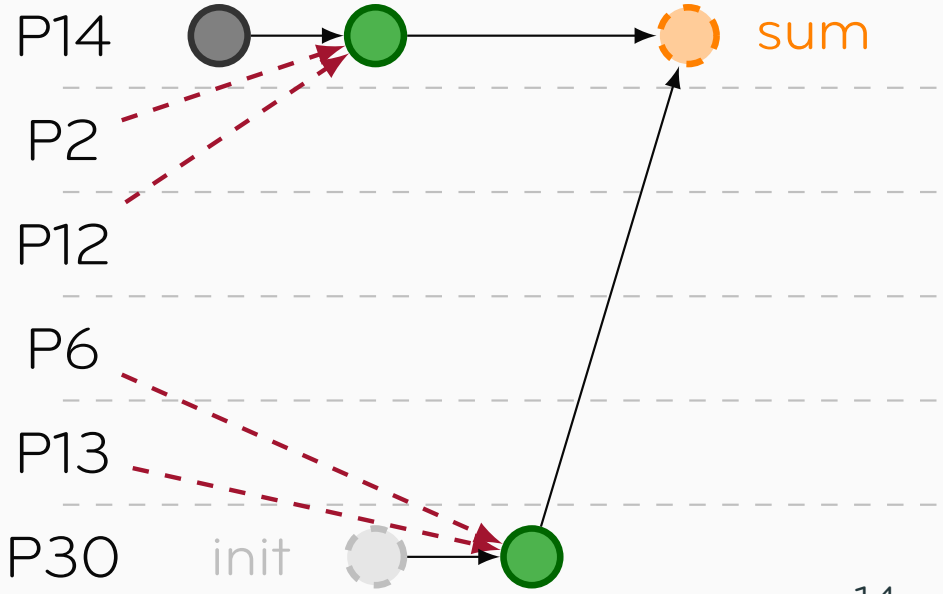
    end do
  end do
end do
```



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,
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                       B_{l,j}:R,
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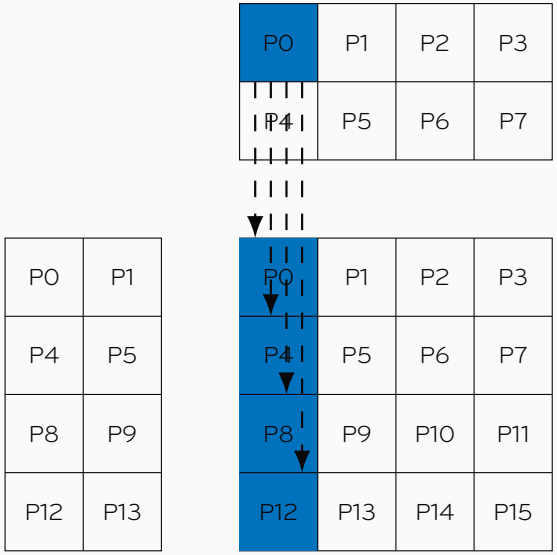
                       task_map[i,j,l])
    end do
  end do
end do
```



Advanced model MX

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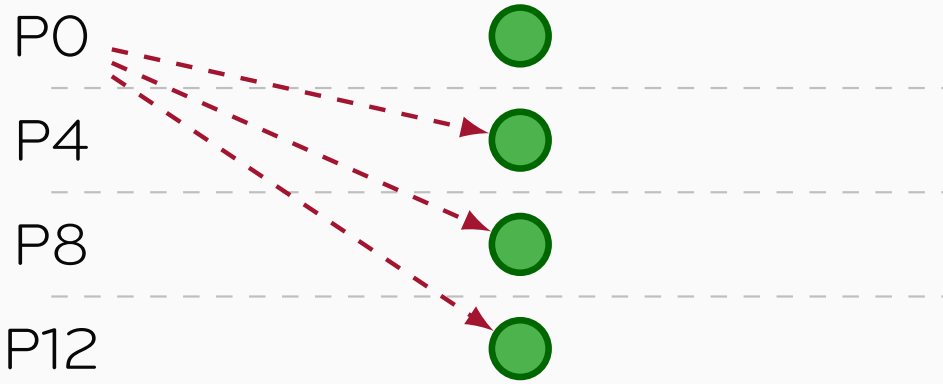
- MX-1 Explicit task mapping
- MO-2 Comms. inferred
- MX-3 Implicit reduction pattern



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,
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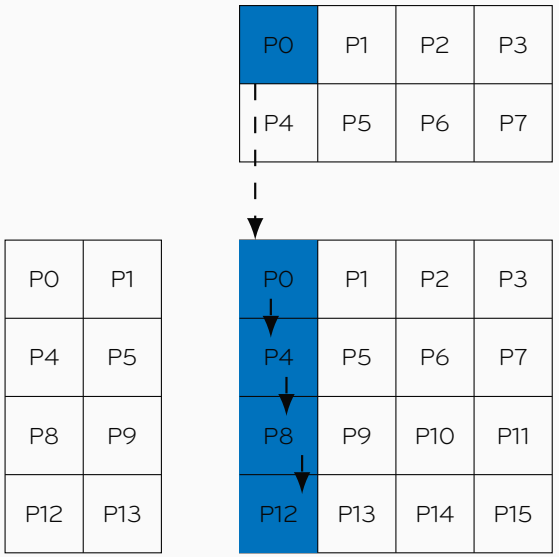
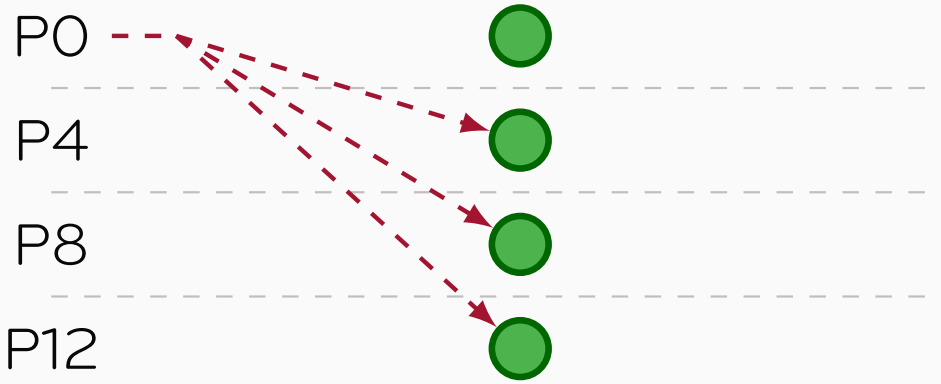
    end do
  end do
end do
```



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

```
!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,
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                       task_map[i,j,l])
    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

EXPERIMENTAL RESULTS

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
    - Synchronous MPI + seq. BLAS
    - 2D A,B,C-stationary
  - `slate` – OpenMPI 4.0.5, 1 MPI / node
    - MPI + OpenMP with `task` + seq. BLAS
    - 2D A,C-stationary with lookahead
  - `chameleon` – newMadeleine, 1 MPI / node
    - StarPU with explicit comms. management + seq. BLAS
    - 2D C-stationary pipelined with lookahead
- **Hardware**: Très Grand Centre de Calcul (TGCC)
  - **Irène - Skylake** Infiniband EDR, 4x links
    - Dual-processor Intel Skylake 8168 @ 2.7 GHz
    - 24 cores per processor, 192 GB DDR4 memory
  - **Irène - Rome** Infiniband HDR100, 2x links
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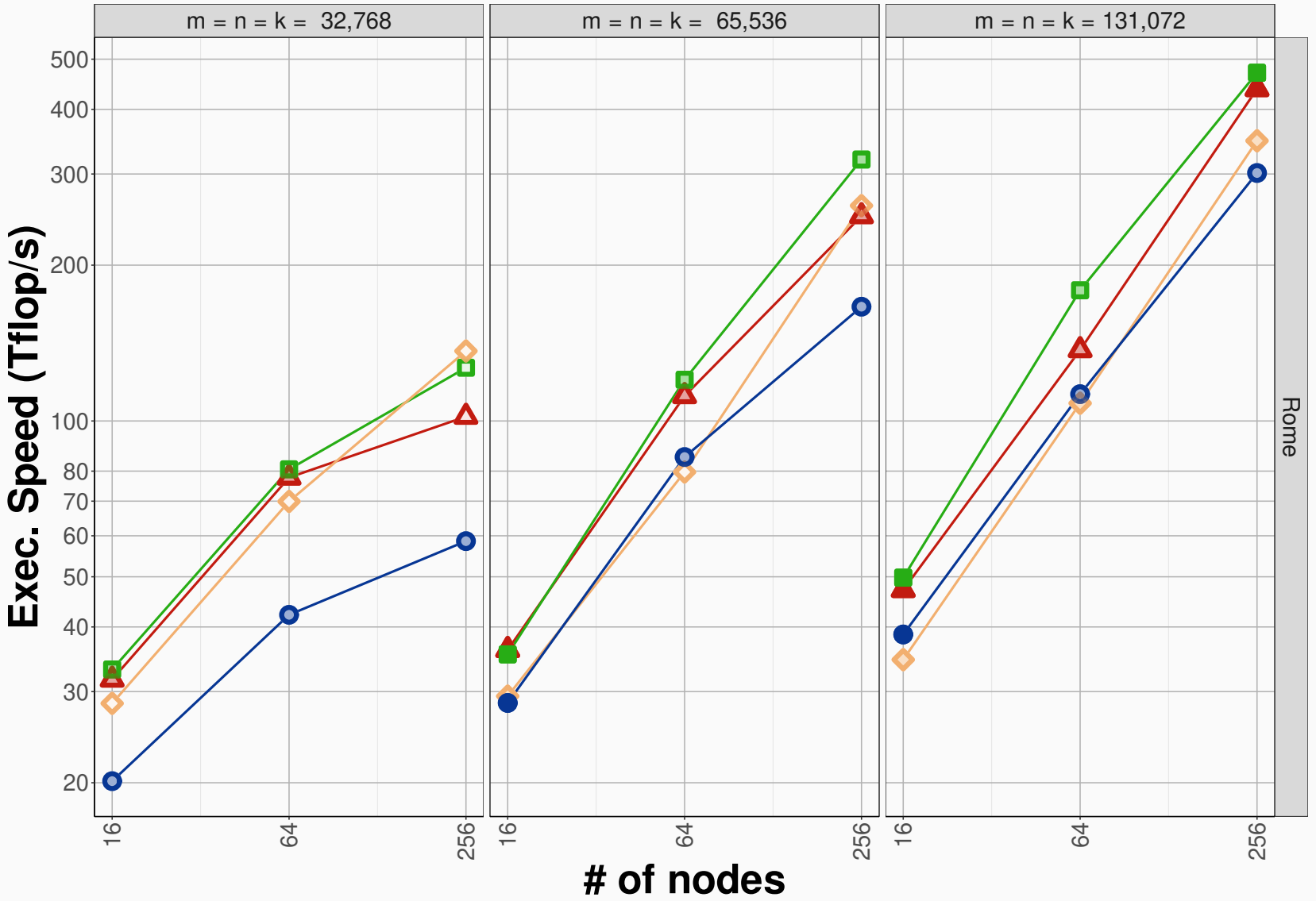
Rome (up to 32,768 cores) – square matrices, DGEMM



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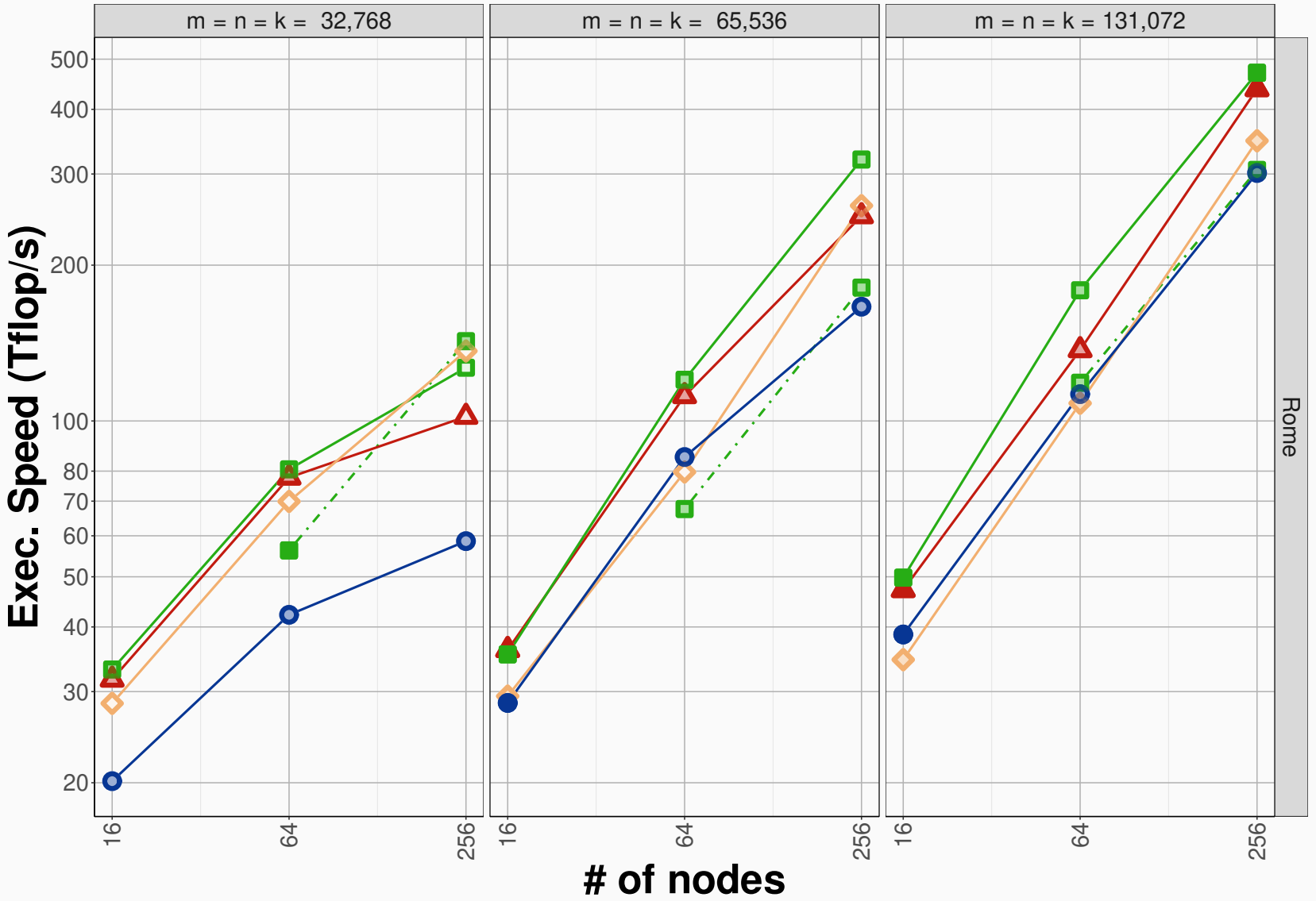
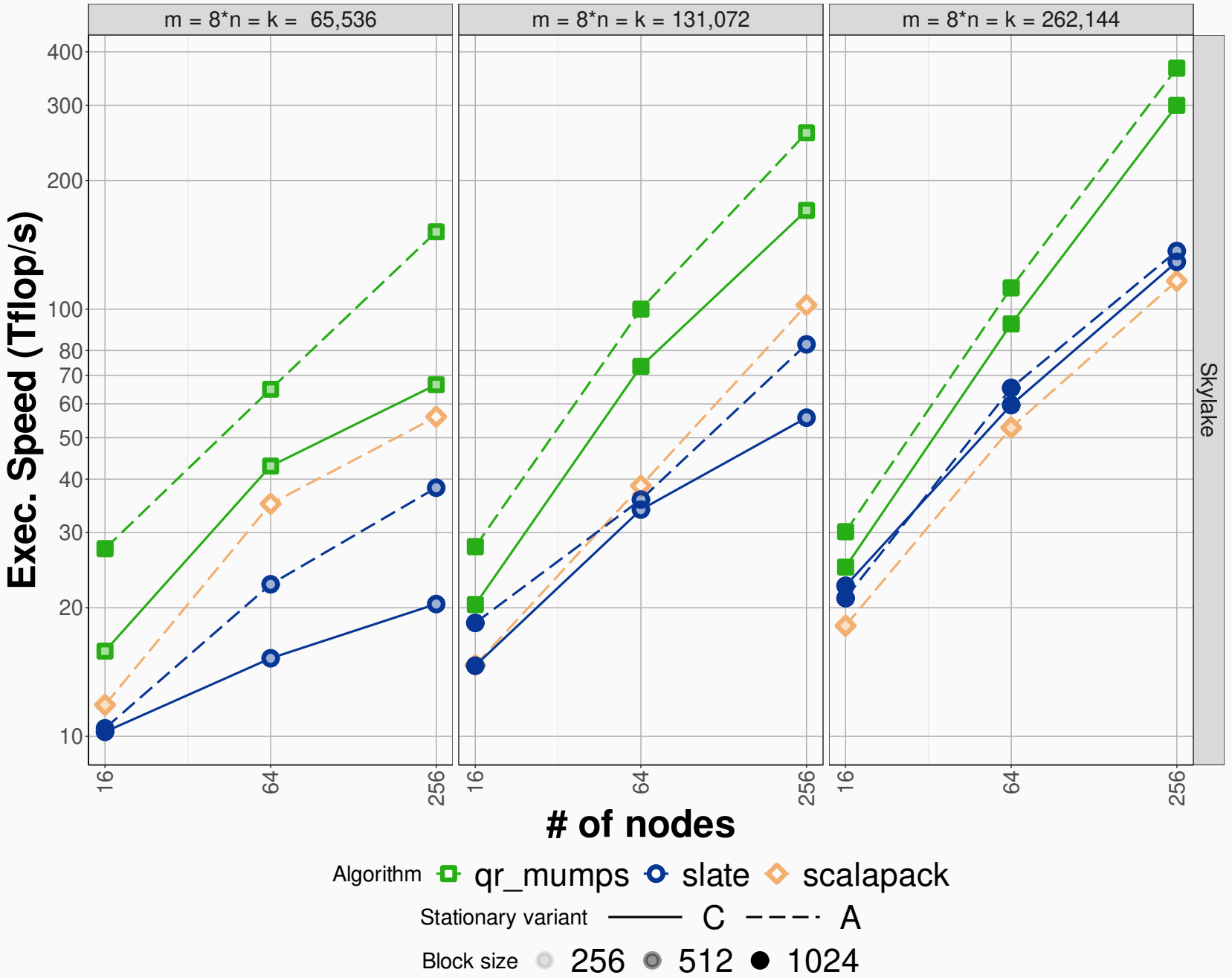


Skylake (up to 12,288 cores) – large A, DGEMM



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

- Studying SYMM in the context of a scientific application
  - In collaboration with O. Beaumont, O. Coulaud, L. Eyraus-Dubois, A. Franc, R. Peressoni, F. Pruvost, M. Vérité
- Studying the scheduling of communication patterns in GEMM
  - In collaboration with O. Beaumont, A. Denis, L. Eyraus-Dubois, E. Jeannot, M. Vérité, P. Swartvagher

Future work

We want to address more distributed-memory scalable algorithms

- Dense **2.5D** Cholesky, LU **factorizations**
- Sparse factorizations

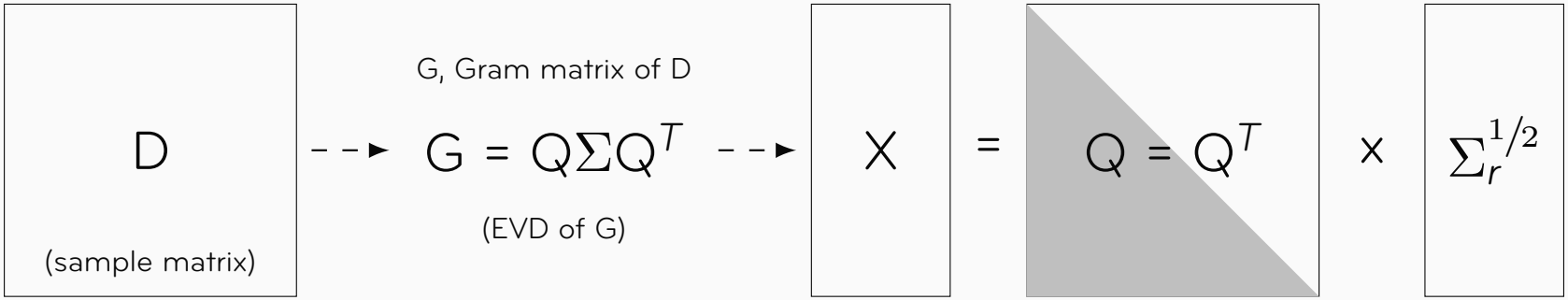
However, we need further **extensions** to the current programming model

- **Replication of computation** as required by **state-of-the-art 2.5D** algorithms
- **All-reduce pattern** to ensure **stability** through tournament pivoting
- **Memory-awareness** to ensure an algorithm will **not exceed** a user-defined **memory constraint**

ON-GOING WORK

Symmetric Matrix Multiplication (SYMM) – application

Our versatile approach is of interest in the **`Fast Methods for Randomized numerical algebra`** (FMR) data mining library.

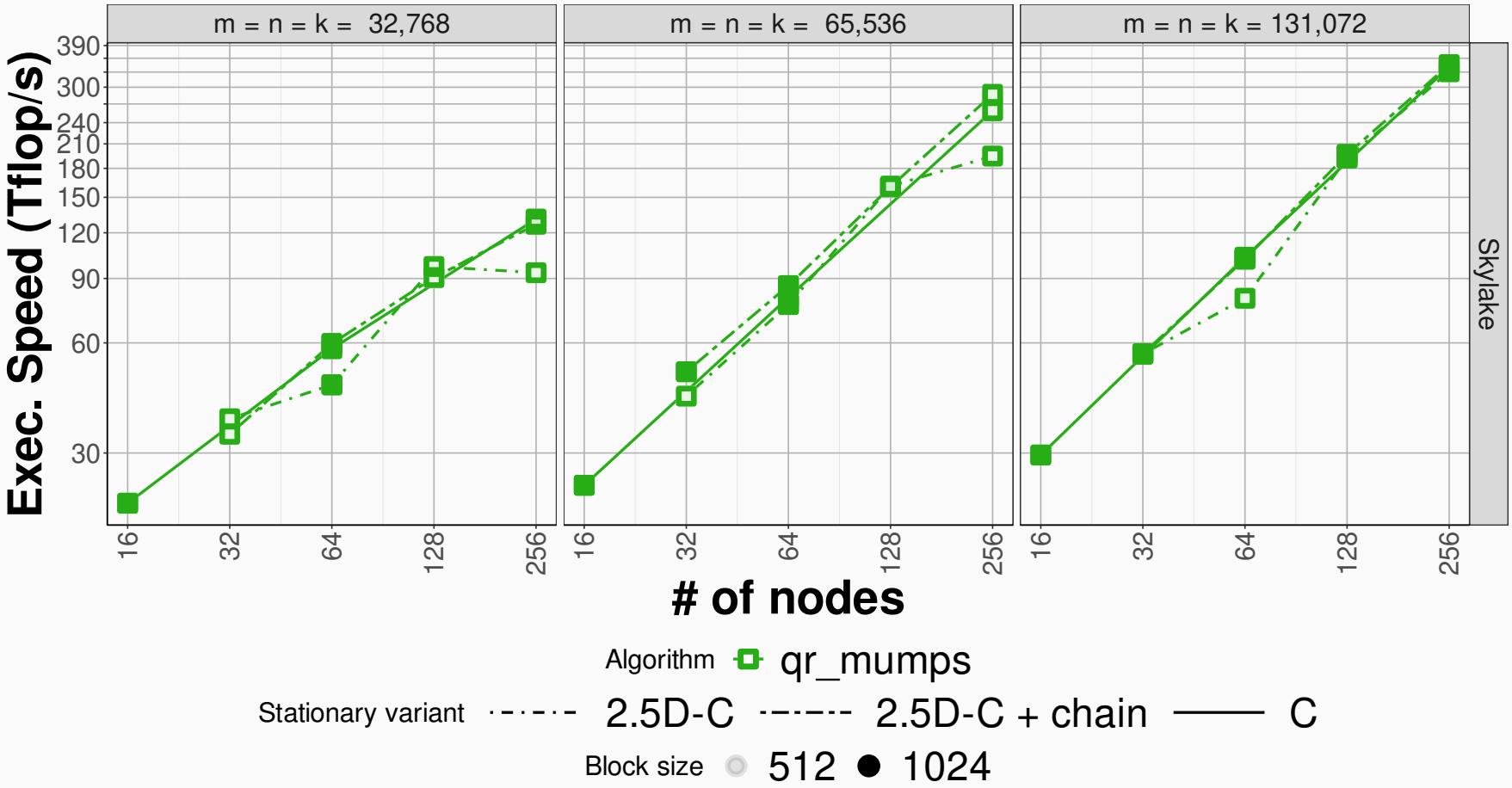


- **A-stationary algorithm**: involved matrices are disproportionate
- **distribution-agnosticism**: to deploy *symmetric distributions*

⇒ In collaboration with:
Olivier Beaumont, Olivier Coulaud, Lionel Eyraus-Dubois, Alain Franc, Romain Peressoni, Florient Pruvost, Mathieu Vérité

Extensive study on communication ordering for GEMM

Experiments questionning the scheduling of communications



⇒ In collaboration with:

Olivier Beaumont, Alexandre Denis, Lionel Eyraus-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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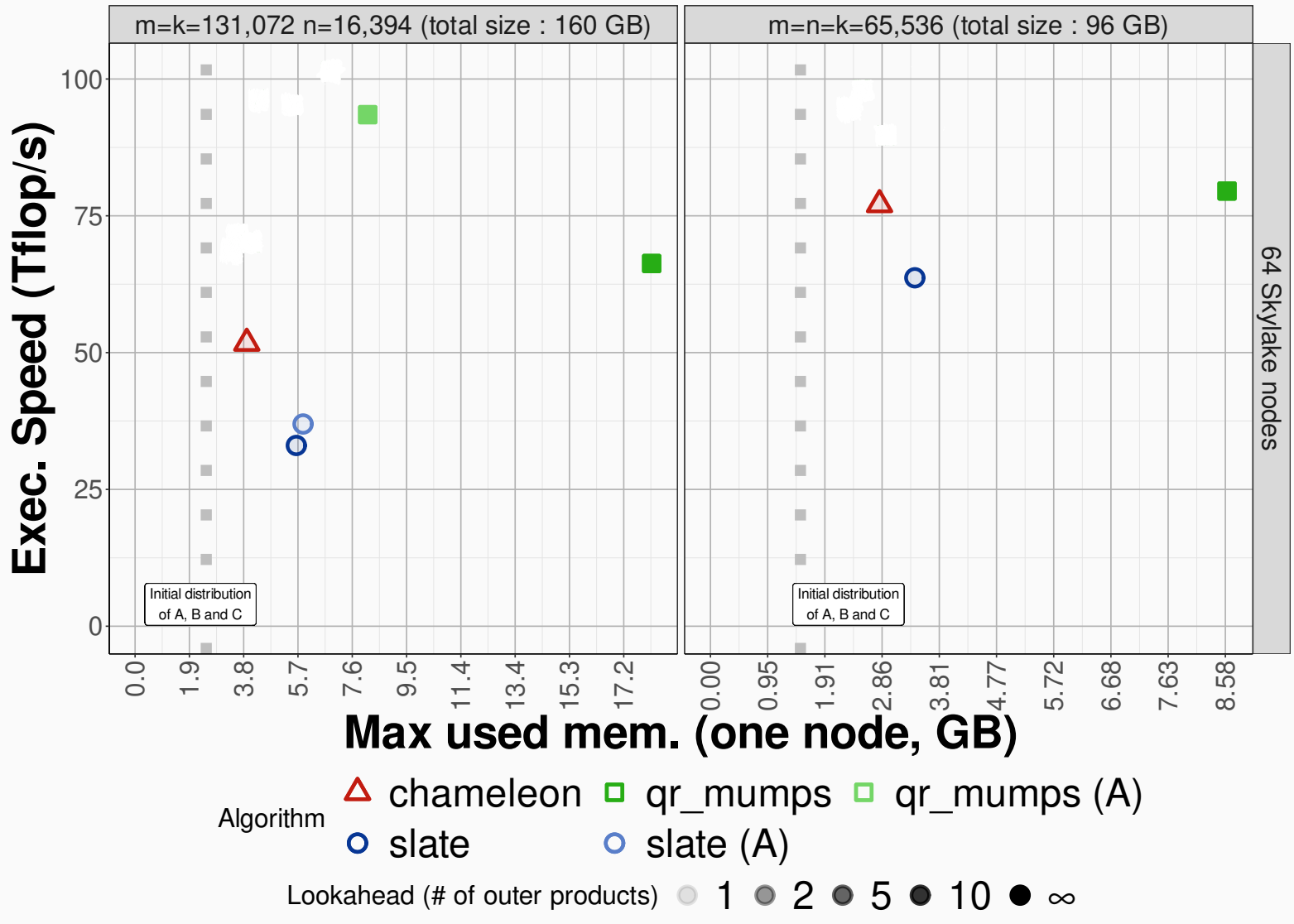
BACKUP SLIDES

Memory Consumption Concern - experiment

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

Task window mechanisms can help limit memory consumption



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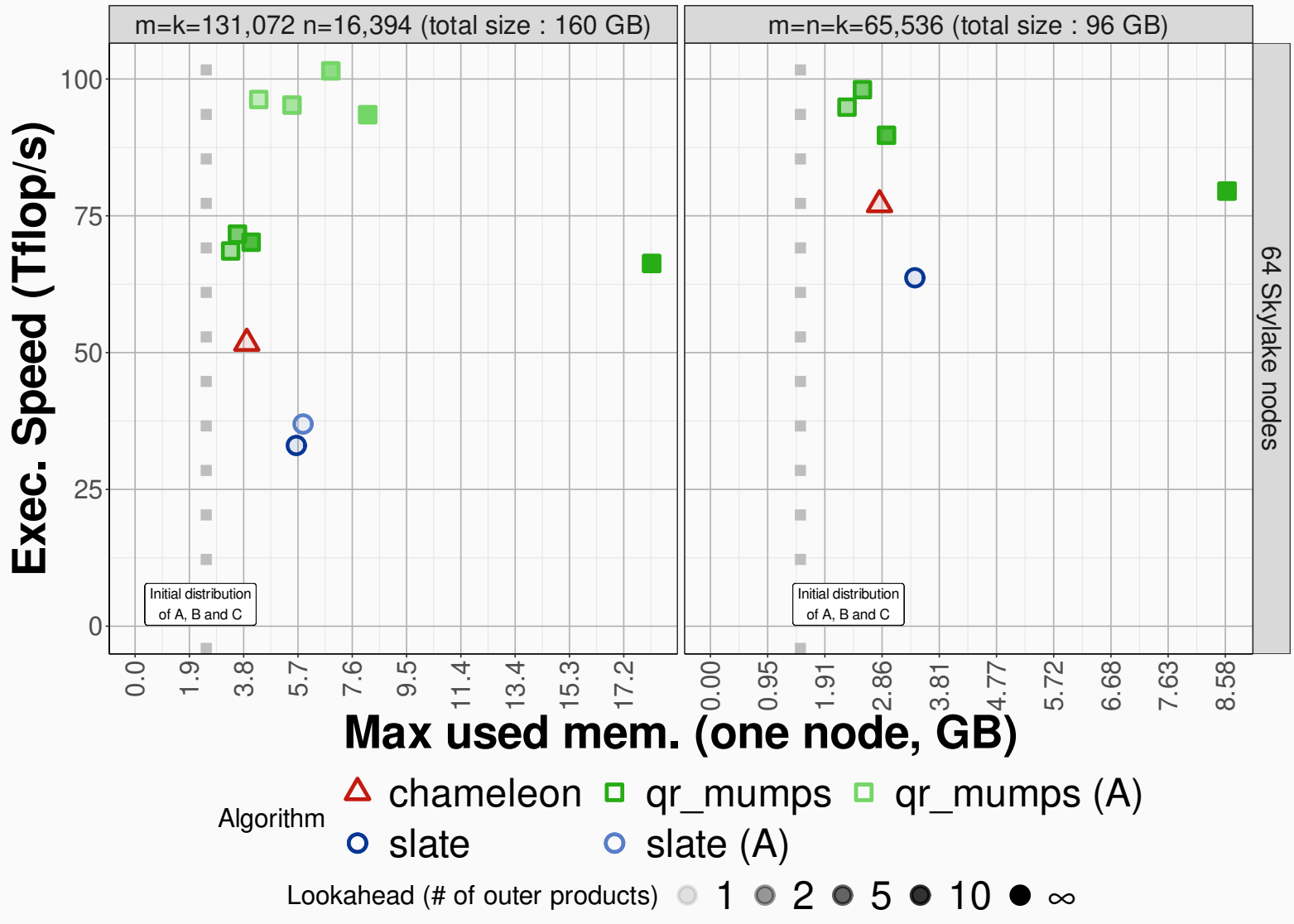


Some common operations are done before switching on the `stat` parameter:

- 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)
```

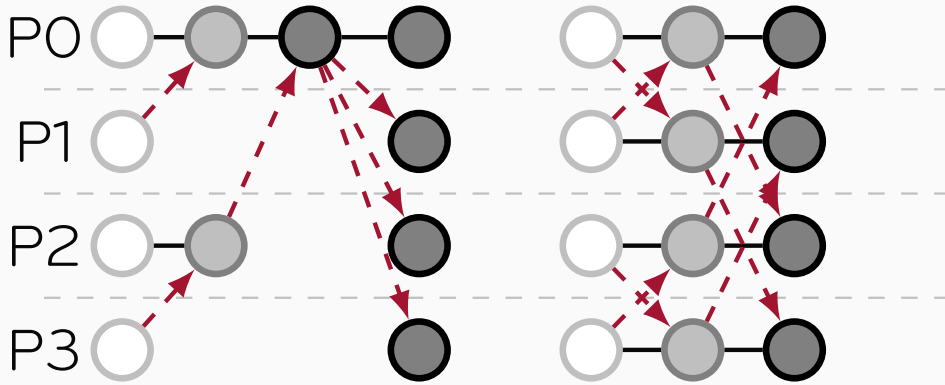
⇓

```
! 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



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.

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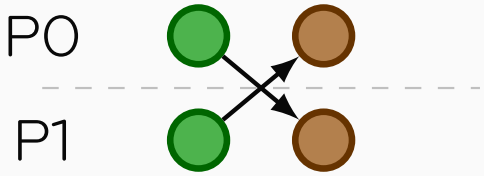

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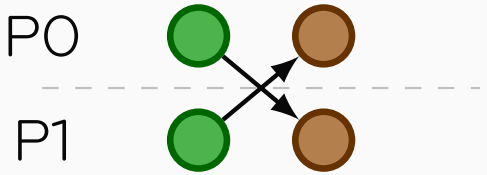

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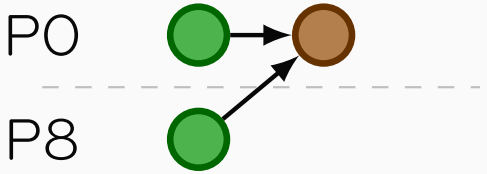

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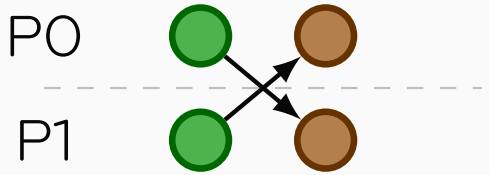

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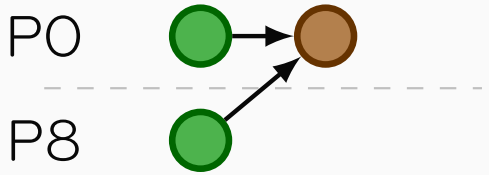

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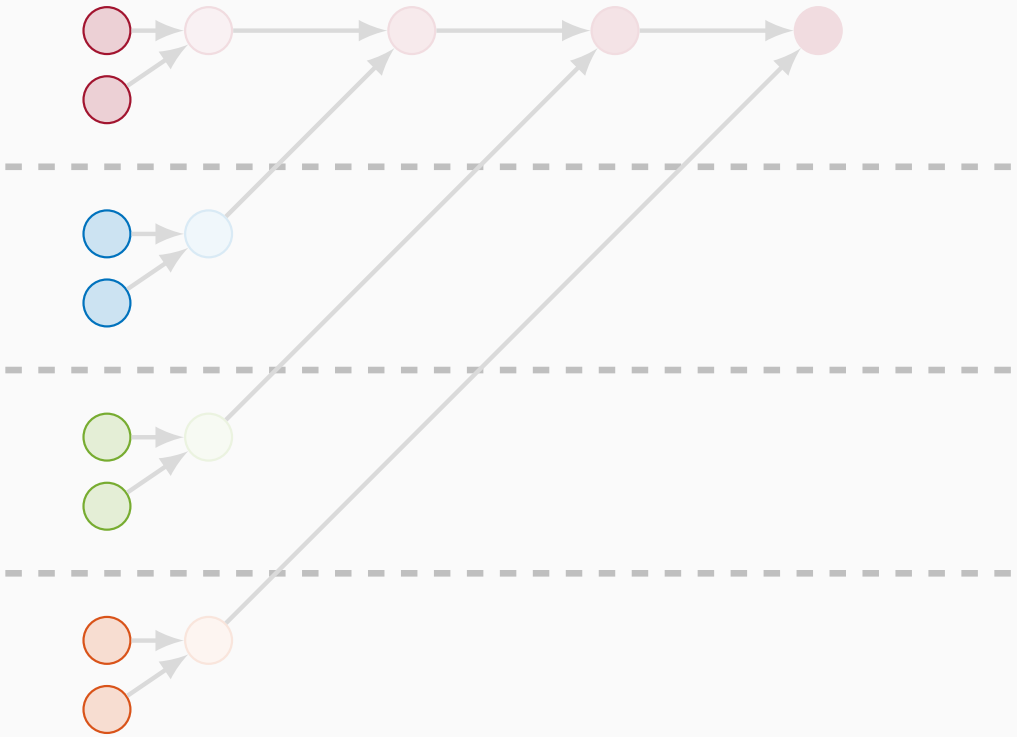
Features of StarPU – 1.3

- `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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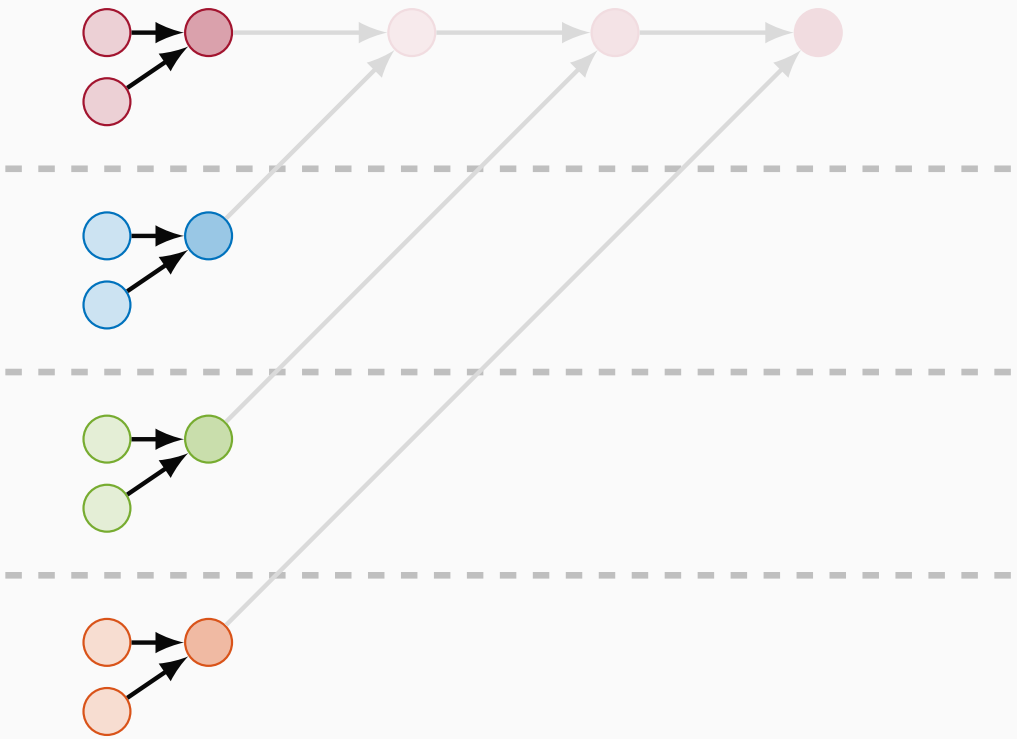

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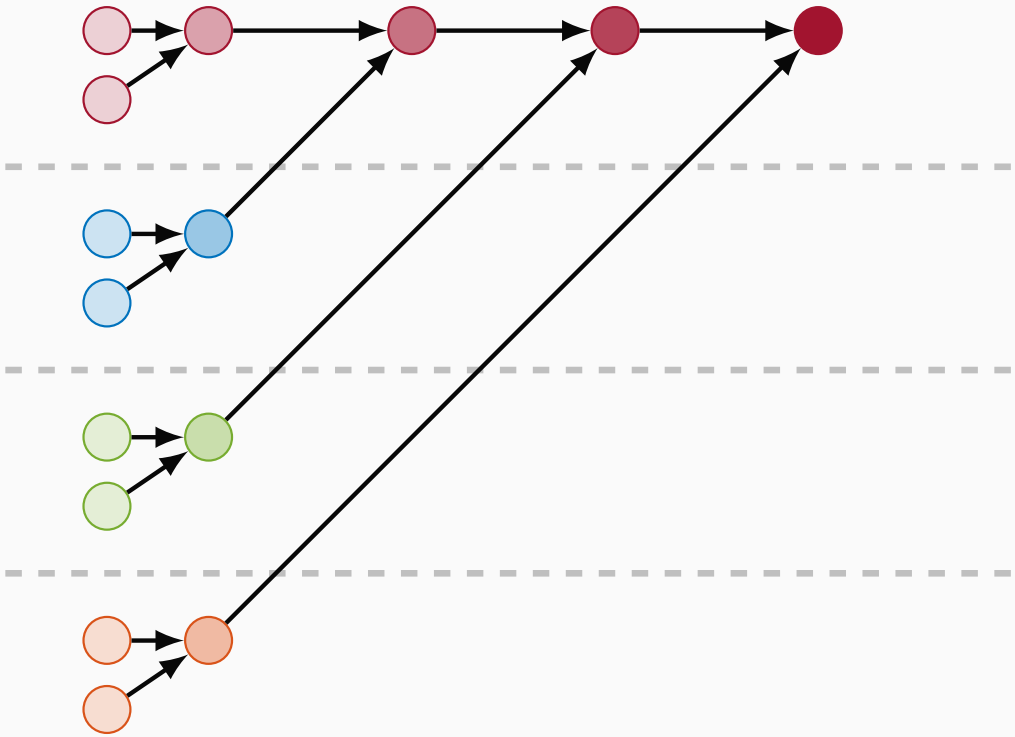

Features of StarPU – our contribution

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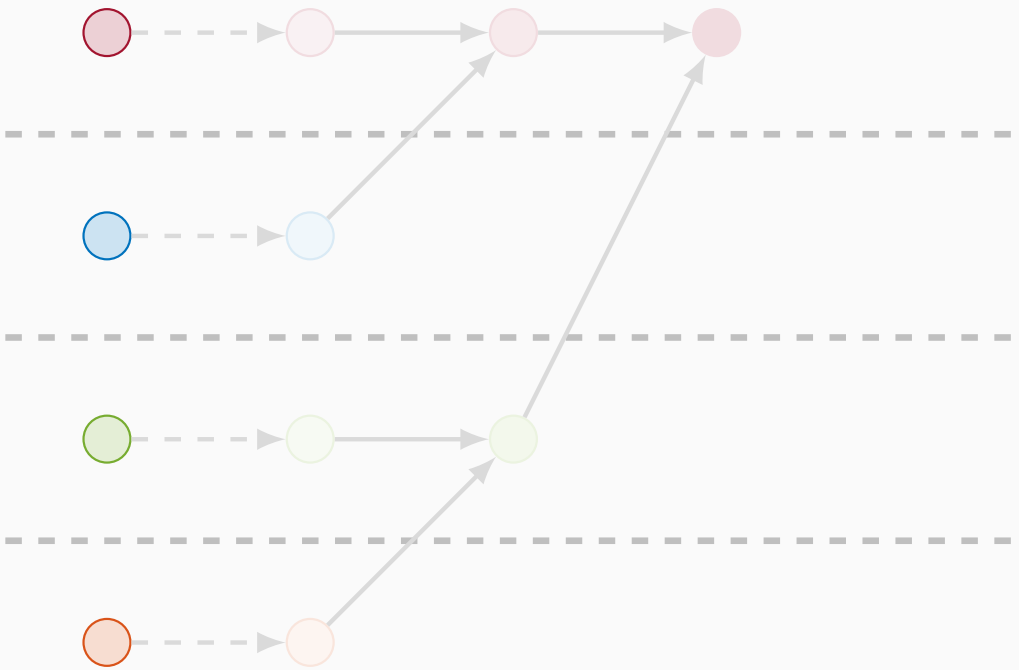

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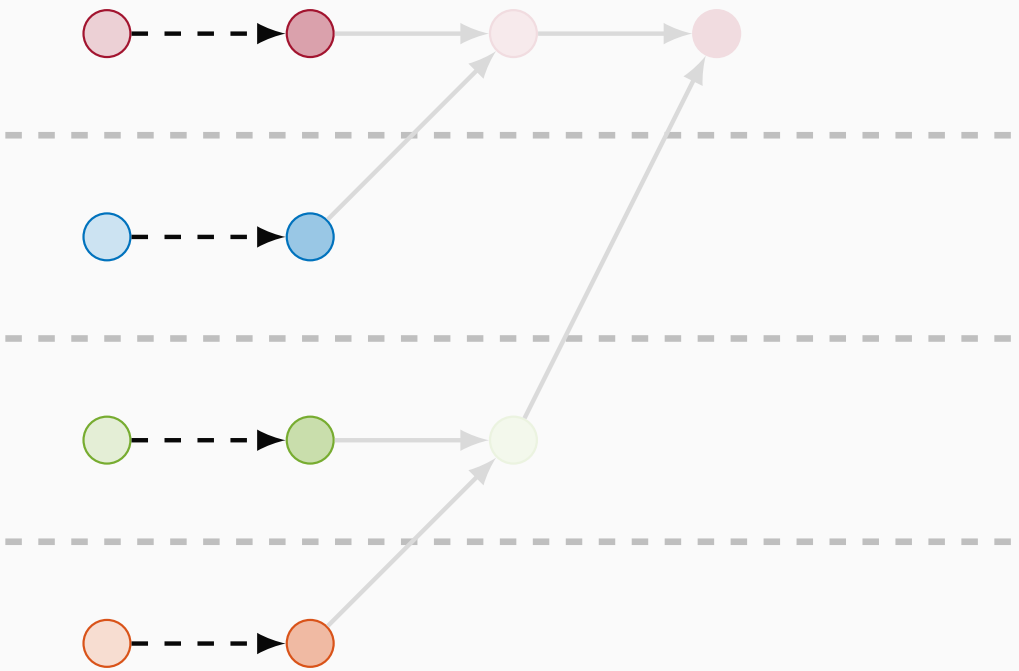

X

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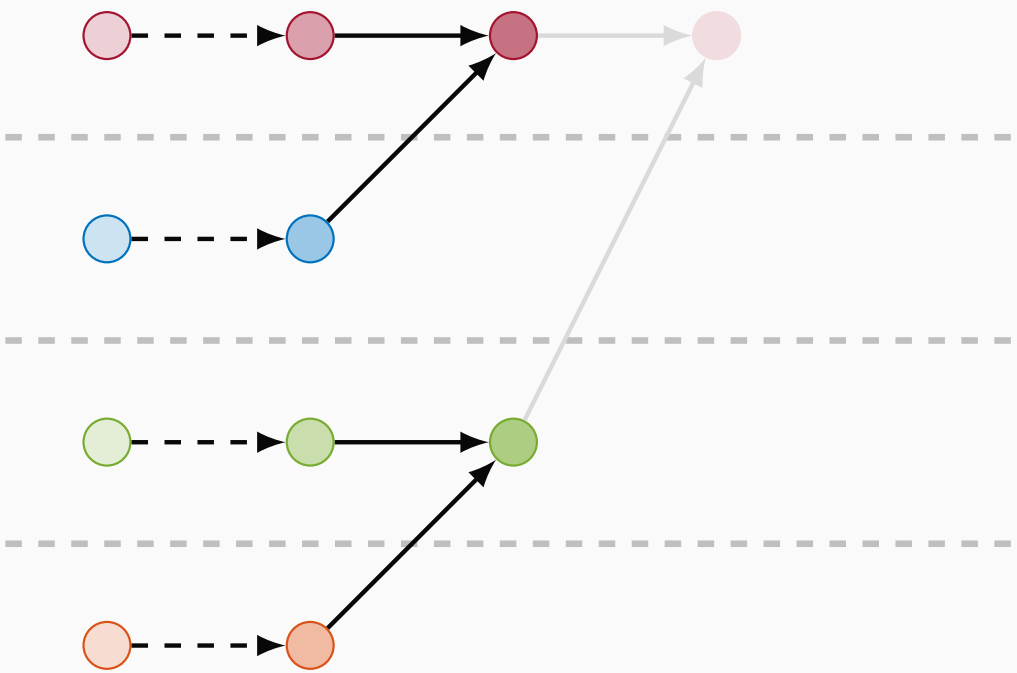

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