TASK-BASED PARALLEL PROGRAMMING FOR SCALABLE ALGORITHMS AND ILLUSTRATION WITH MATRIX MULTIPLICATION JCAD 2024

Antoine Jégo

Supervised by Alfredo Buttari, Emmanuel Agullo & Abdou Guermouche

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BACKGROUND

COMPUTER ARCHITECTURE AND PROGRAMMING MODELS

Supercomputers evolution



Classical approach



Runtime system approach



Complex supercomputers ⊕ Advanced scalability techniques ↓ Complex software

General-purpose runtimes

- High-level interface
- Data management
- Heterogeneity management

Classical approach



Runtime system approach



Complex supercomputers ⊕ Advanced scalability techniques ↓ Complex software

General-purpose runtimes

- High-level interface
- Data management
- Heterogeneity management



- Approach validated on heterogeneous single-node machine
 - SOLHAR among multiple scientific projects
- Multiple ways to program the high-level description of the DAG
 - Parametrized Task Graph (PTG): PaRSEC
 - Sequential Task Flow (**STF**): PaRSEC, StarPU

° ...

SEQUENTIAL TASK FLOW MODEL





Algorithm 1: Sequential blocked GEMM.

1 for $i = 1 \dots m$ do

$$\begin{array}{c|c} \mathbf{2} & \mathbf{for} \ j = 1 \dots n \ \mathbf{do} \\ \mathbf{3} & \mathbf{for} \ l = 1 \dots k \ \mathbf{do} \end{array}$$

$$\mathbf{4} \quad | \quad | \quad C_{ij} \mathrel{+}= A_{il} \cdot B_{lj}$$

Algorithm 2: Shared-memory STF GEMM.

```
1 for i = 1...m do

2 for j = 1...n do

3 for l = 1...k do

4 insert_task
```

5 task_wait()

Sequential Task Flow Model





Algorithm 1: Sequential blocked GEMM.

1 for i = 1 ... m do

2 for
$$j = 1 \dots n$$
 do
3 for $l = 1 \dots k$ do

$$| | C_{ij} + = A_{il} \cdot B_{lj}$$

Algorithm 2: Shared-memory STF GEMM.

4~

1 for
$$i = 1...m$$
 do
2 | for $i = 1...n$

5 task_wait()

3

4

Pros of runtime systems:

- Increased portability
- Improved separation of concerns

Pros of the STF model:

- Productive
- Clear translation from sequential

In practice, scientific computing software use **hand-tuned**, **application-tailored advanced** communication patterns, data layouts, workload mappings, ...

Is STF expressive enough to transparently schedule these techniques and reach existing and new scalable algorithms ?

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Algorithm 3: STF GEMM.

1 for
$$i = 1...m$$
 do
2 for $j = 1...n$ do
3 for $l = 1...k$ do
4 insert_task(gemm, ?

ScaLAPACK GEMM $\mathcal{O}(1k)$ lines of code legacy package

Three portable nested loops

Contributions

- Extension of the STF programming model
 - Data replication features (reduction, replication)
 - Validated over dense linera algebra operations (GEMM, SYMM, POTRF)

STF SCALABLE MATRIX-MATRIX MULTIPLICATION

Scalable Universal Matrix Multiplication Algorithms (SUMMA)

A-, B- and C-stationary depending on matrices' dimensions.



SUMMA – 2D C-stationary¹

• 2D block-cyclic distribution



• owner of C computes

• Communications

- row-wise broadcast of A
- $\circ~$ column-wise broadcast of B $\,$

¹R. v. d. Geijn and Watts, 1997



SUMMA – 3D C-stationary²

- 2D block-cyclic (first layer)
- owner of C's aisle (across layers) compute

- row-wise scatter+broadcast of A
- column-wise scatter+broadcast of B
- $\circ~$ aisle-wise reduce of C







SUMMA – 3D C-stationary²

- 2D block-cyclic (first layer)
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- $\circ~$ aisle-wise reduce~of~C



Algorithm 4: Baseline 2D GEMM.

1 for $i = 1 \dots m$ do 2 for $j = 1 \dots n$ do 3 for $l = 1 \dots k$ do 4 linsert_task (gemm, $A_{il}: \mathbb{R}, B_{lj}: \mathbb{R}, C_{ij}: \mathbb{RW}$)





Baseline model^a

- 1. Data mapping
- 2. Task mapping **inferred** from data mapping
- 3. Point-to-point comms. **inferred** from task mapping

^aAgullo, Aumage, Faverge, Furmento, Pruvost, Sergent, and Thibault, 2017.

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Baseline STF model cannot **productively** provide an expression of SUMMA algorithms

- ✗ Task mapping is bound to data mapping
- X Point-to-point communications patterns are inefficient
- X Reduction patterns would burden the expression



Key features – task mapping

Algorithm 5: 3D GEMM (I/III).

1 for i = 1...m do 2 for j = 1...m do 3 for l = 1...k do 4 linsert_task (gemm, $A_{il}:R, B_{lj}:R, C_{ij}:RW$)

- 1. Data mapping
- 2. Implicit task mapping
- 3. Point-to-point comms. inferred from task mapping

Key features – task mapping

Algorithm	5:	ЗD	GEMM	(1)	/111).
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1 f	1 for $i=1\dots m$ do								
2	f	$r j = 1 \dots n$ do							
3		for $l=1\dots k$ do							
4		rank = map(i,j,l,stat,s)							
5		insert_task (gemm, A_{il} :R, B_{lj} :R,							
		C _{ij} :RW, rank :ON_RANK)							

- 1. Data mapping
- 2. Explicit task mapping
- 3. Point-to-point comms. inferred from task mapping

Key features - collective transfers

1	1 for $i = 1 \dots m$ do								
2	2 for $j = 1n$ do								
3	for $l=1\ldots k$ do								
4	rank = map(i,j,l,stat,s)								
5	$insert_task (gemm, A_{il}:R, B_{lj}:R,$								
	C _{ij} :RW, rank:ON_RANK)								



- 1. Data mapping
- 2. Explicit task mapping
- 3. Point-to-point comms. inferred from task mapping



KEY FEATURES - COLLECTIVE TRANSFERS

	Algorithm 6: 3D GEMIM (II/III).									
1	1 for $i = 1 \dots m$ do									
2	for $j = 1 \dots n$ do									
3	for $l=1\dots k$ do									
4	rank = map(i,j,l,stat,s)									
5	$\texttt{insert_task}$ (gemm, A_{il} :R, B_{lj} :R,									
	C _{ij} :RW, rank:ON_RANK)									



- 1. Data mapping
- 2. Explicit task mapping
- 3. Collective communications dynamically detected^a

^aDenis, Jeannot, Swartvagher, and Thibault, 2020.

Key features - reduction operations

Algorithm 7: 3D GEMM (III/III).

1 submit_initilization_tasks() 2 for $i = 1 \dots m$ do 3 for $j = 1 \dots m$ do 4 for $l = 1 \dots k$ do 5 l rank = map(i,j,l,stat,s) 6 l rinsert_task (gemm, A_{ij} :R, B_{ij} :R, $C_{ij}^{(rank)}$:RW, rank:ON_RANK) 7 submit_reduction_tasks()



- 1. Data mapping
- 2. Explicit task mapping
- 3. Collective communications dynamically detected
- 4. Explicit reduction pattern

Key features - reduction operations

Algorithm 7: 3D GEMM (III/III).

1	bind_methods(C,redux,init)								
2	2 for $i=1\ldots m$ do								
3	fo	${f r}j=1\dots n$ do							
4		for $l=1\dots k$ do							
5		rank = map(i,j,l,stat,s)							
6		$insert_task (gemm, A_{il}:R, B_{lj}:R,$							
		C_{ij} :RANK_REDUX,							
		rank:ON_RANK)							



- 1. Data mapping
- 2. Explicit task mapping
- 3. Collective communications dynamically detected
- 4. Implicit reduction pattern

STF⁺ 3D GEMM expression

Algorithm 8: 3D GEMM.

1	bind_methods(C,redux,init)								
2	e for $i=1\dots m$ do								
3	for $j = 1 \dots n$ do								
4		for $\textit{I} = 1 \dots k$ do							
5		rank = map(i,j,l,stat,s)							
6		insert_task (gemm, A_{il} :R, B_{lj} :R,							
		C_{ij} :RANK_REDUX,							
		rank:ON_RANK)							

Conclusion I

Suitably extended STF model can **portably** express scalable GEMM algorithms.

s this approach scalable in practice ?

Advanced model = STF*

- 1. Data mapping
- 2. Explicit task mapping
- 3. Collective communications dynamically detected
- 4. Implicit reduction pattern

STF⁺ 3D GEMM expression

Algorithm 8: 3D GEMM.

1	bind_methods(C,redux,init)								
2	2 for $i=1\ldots m$ do								
3	for $j = 1 \dots n$ do								
4	f	for $l=1\ldots k$ do							
5		rank = map(i,j,l,stat,s)							
6		insert_task (gemm, A_{il} :R, B_{lj} :R,							
		C_{ij} :RANK_REDUX,							
		rank:ON_RANK)							

Conclusion I

Suitably extended STF model can **portably** express scalable GEMM algorithms.

Is this approach scalable in practice ?

Advanced model = STF*

- 1. Data mapping
- 2. Explicit task mapping
- 3. Collective communications dynamically detected
- 4. Implicit reduction pattern

Runtime system used is StarPU – extended with improved reduction features.

STF⁺ GEMM has been implemented in qr_mumps.

software package	programming model	С	2D A	В	3D all	GPU
Chameleon 1.1	STF ^X , StarPU 1.3	 ✓ 	X	X	×	 Image: A second s
SLATE	MPI+OpenMP	 ✓ 	1	X	×	\checkmark
DPlasma	PTG, PaRSEC	 Image: A start of the start of	 Image: A second s	√	X	1
ScaLAPACK	SPMD, BLACS	 Image: A start of the start of	1	\checkmark	X	X
Elemental	SPMD	 Image: A start of the start of	\checkmark	\checkmark	×	X
this work	STF [↓] , StarPU 1.4	 Image: A start of the start of	1	 Image: A start of the start of	 Image: A second s	\checkmark

Machines hosted inside the Très Grand Centre de Calcul (TGCC).

A. Irène-Rome AMD Rome 7H12 2.6 GHz

- 2,292 128-cores nodes with Infiniband HDR100 interconnect
- \circ $R_{\rm peak} = 11.75 \ {\rm PFlop/s}$
- 256GB DDR4 RAM per node
- B. Irène-Skylake Intel Skylake 8168 2.7 GHz
 - 1,656 48-cores nodes with Infiniband EDR interconnect
 - \circ R_{peak} = 6.86 PFlop/s
 - 192GB DDR4 RAM per node

Overall about 1 million CPU hours consumed.

EXPERIMENTS - PERFORMANCE (C-STAT)



Conclusion II

STF⁺ offers competitive performance w.r.t reference libraries

EXPERIMENTS - PERFORMANCE (C-STAT)



Conclusion II

STF⁺ offers competitive performance w.r.t reference libraries

EXPERIMENTS - PERFORMANCE (A-STAT)



Conclusion III

STF⁺ brings versatility together with performance



EXPERIMENTS – PERFORMANCE (A-STAT)



Conclusion III

STF⁺ brings versatility together with performance





Memory consumption control through limits on tasks' flow





Memory consumption control through limits on tasks' flow.





Conclusion IV

STF⁺ incorporates tunable indirect method to control memory consumption





Conclusion IV

STF⁺ incorporates tunable indirect method to control memory consumption



CONCLUSIONS

STF⁺ assessment over linear algebra operations

I Suitably extended STF model can portably express scalable GEMM algorithms
 II STF⁺ offers competitive performance w.r.t reference libraries
 III STF⁺ brings versatility together with performance

Additional contributions (not discussed here)

- Implementation of scalable SYMM, POTRF algorithms
- Implementation of a communication-avoiding 2D 5-points stencil prototype



Software contributions

- Implementation of additional features in StarPU
 - Distributed-memory reduction patterns
- Implementation of dense scalable routines in qr_mumps

Transfer

- Chameleon 1.3
 - $\circ~$ Used by INRAE colleagues to analyse biodiversity datasets

