Communication Avoiding and Overlapping for Numerical Linear Algebra

Evangelos Georganas<sup>1</sup>, Jorge González-Domínguez<sup>2</sup>, Edgar Solomonik<sup>1</sup>, Yili Zheng<sup>3</sup>, Juan Touriño<sup>2</sup>, Katherine Yelick<sup>1,3</sup>

<sup>1</sup>Department of Electrical Engineering and Computer Sciences, UC Berkeley <sup>2</sup>Department of Electronics and Systems, University of A Coruña <sup>3</sup>Lawrence Berkeley National Laboratory

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#### Introduction

Linear algebra algorithms Performance modeling Conclusions Communication is Expensive Communication avoidance vs Overlapping CA and CO in Linear Algebra

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#### Introduction

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Communication is Expensive Communication avoidance vs Overlapping CA and CO in Linear Algebra

#### Communication is Expensive

#### Communication has two components:

- **Bandwidth cost:** # of words moved / bandwidth
- ► Latency cost: # messages × latency

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Communication exists in **memory hierarchy** and **network** Things are bad and **getting worse**:

#### flop time $\ll 1/\textit{bandwidth} \ll \textit{latency}$

Annual improvements [FOSC]					
Flop time		Bandwidth	Latency		
	Network	26%	15%		
59%	DRAM	23%	5%		

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	Network	26%	15%		
59%	DRAM	23%	5%		

Communication is also expensive in energy

Communication is Expensive Communication avoidance vs Overlapping CA and CO in Linear Algebra

#### Communication Avoidance vs Overlapping

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#### Communication Avoidance vs Overlapping

Two techniques to minimize the impact of communication: 1. **Communication Avoidance (CA):** 

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  - Leads to provably optimal algorithms

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#### 2. Communication Overlapping (CO):

- Reduces the impact of each communication event by overlapping it with computation
- Hides bandwidth and/or latency cost
- Most effective if communication & computation are balanced

## CA and CO in Linear Algebra

- ► We studied these techniques in three Linear Algebra routines:
  - Matrix Multiplication (SUMMA and Cannon's algorithms)
  - Cholesky factorization
  - Triangular Solve

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Optimizations Algorithm	Overlapping	Avoidance	Overlapping & Avoidance
SUMMA	PRIOR	PRIOR	
Cannon's	PRIOR	PRIOR	
Cholesky	PRIOR		
TRSM	PRIOR		

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Optimizations Algorithm	Overlapping	Avoidance	Overlapping & Avoidance
SUMMA	PRIOR	PRIOR	NEW
Cannon's	PRIOR NEW: One sided communication	PRIOR NEW: One sided communication	NEW
Cholesky	PRIOR	NEW	NEW
TRSM	PRIOR	NEW*	NEW*

\*Uses replication but not communication optimal

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#### Three major questions arise:

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- 3. Can we explain the behavior of CA and CO under different situations?

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### CA and CO in Linear Algebra

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Matrix Multiplication Cholesky factorization Triangular Solve (TRSM)

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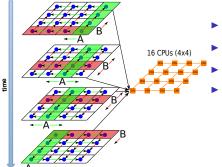
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# Conclusions Conclusions

Matrix Multiplication Cholesky factorization Triangular Solve (TRSM)

#### 2D Matrix Multiplication (SUMMA) [Van De Geijn and Watts 97]



- Outer product form of Mat Mul
- Partitions A, B and C in 2 dimensions

Row and column broadcast on 2D grid

- Costs:
  - $O(n^3/p)$  flops
  - $O(n^2/\sqrt{p})$  words moved
  - $O(\sqrt{p})$  messages

Matrix Multiplication Cholesky factorization Triangular Solve (TRSM)

### 2D Matrix Multiplication with CO (SUMMA)

- We overlap the broadcasts of next iteration with the local Mat.Mul computation of current iteration
- Theoretically the execution time becomes t<sub>exec</sub> = O(max(t<sub>computation</sub>, t<sub>communication</sub>))
- If communication and computation are balanced we can achieve up to 2× speedup
- Additional communication buffers are needed

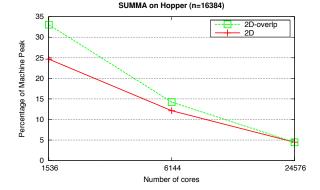
Matrix Multiplication Cholesky factorization Triangular Solve (TRSM)

#### Experimental setup

- Experiments on Hopper, a Cray XE6 system (153,216 cores)
- We will focus on communication-limited problems (i.e. small problems on large machine configurations)
- Strong scaling experiments

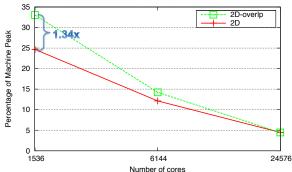
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#### Overlapping yields more benefits at medium scale



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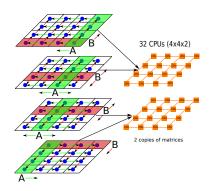


SUMMA on Hopper (n=16384)

- At medium scale where communication and computation are balanced we observe larger benefits (1.34× speedup)
- At large scale overlapping does not help

Matrix Multiplication Cholesky factorization Triangular Solve (TRSM)

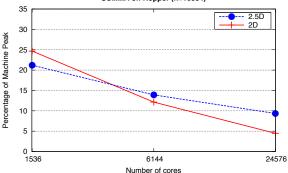
2.5D Matrix Multiplication (SUMMA) [McColl and Tiskin 99], [Solomonik and Demmel 11]



- The 2.5D algorithm uses extra memory to reduce communication
- Each one of the c layers of processors computes a different contribution to the matrix C
- Works for *c* copies,  $c \in [1, p^{1/3}]$
- Costs:
  - $O(n^3/p)$  flops
  - $O(n^2/\sqrt{c \cdot p})$  words moved
  - $O(\sqrt{p/c^3})$  messages

Matrix Multiplication Cholesky factorization Triangular Solve (TRSM)

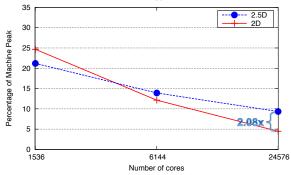
#### Communication avoidance helps a lot at large scale



SUMMA on Hopper (n=16384)

Matrix Multiplication Cholesky factorization Triangular Solve (TRSM)

#### Communication avoidance helps a lot at large scale



SUMMA on Hopper (n=16384)

- ► At large scale avoidance helps a lot (2.08× speedup) (there is a lot of communication to avoid!)
- At medium scale communication avoidance may yield slowdown

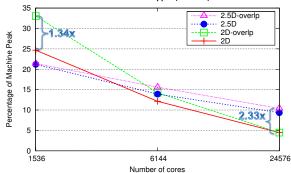
Matrix Multiplication Cholesky factorization Triangular Solve (TRSM)

### 2.5D Matrix Multiplication with CO (SUMMA)

- We overlap the broadcasts of the next iteration with the local Mat.Mul computation of current iteration on each of the c processor layers
- Additional communication buffers are needed on top of the extra memory needed for replication

Matrix Multiplication Cholesky factorization Triangular Solve (TRSM)

### Putting everything together



SUMMA on Hopper (n=16384)

- At medium scale overlapping itself yields best performance
- At large scale combining both techniques pays off

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### Cannon's algorithm

In SUMMA we use collective communication operations

Matrix Multiplication Cholesky factorization Triangular Solve (TRSM)

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Matrix Multiplication Cholesky factorization Triangular Solve (TRSM)

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- The same techniques can be applied for Cannon's algorithm

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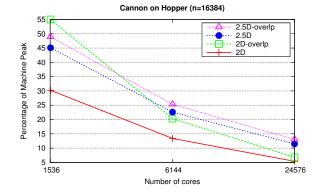
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- Use fast one-sided communication provided by UPC

Matrix Multiplication Cholesky factorization Triangular Solve (TRSM)

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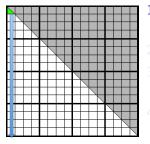


Matrix Multiplication Cholesky factorization Triangular Solve (TRSM)

- Factorize a symmetric positive definite matrix A into  $A = L \cdot L^T$ , where L is lower triangular
- Take advantage of symmetry and store only half of matrix A
- Employ block-cyclic layout for load-balance

Matrix Multiplication Cholesky factorization Triangular Solve (TRSM)

# 2D Cholesky factorization

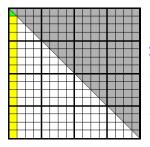


1. Factorize the upper-left (green) block & broadcast it to the column

2. Update via TRSM the (yellow) block column

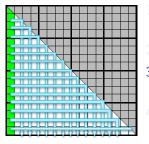
- Broadcast the factorized column in two phases
  & update the trailing matrix (white blocks)
- Continue with the factorization of the second block column and repeat previous steps until all matrix is factorized
- Communication involved is row and column broadcasts
- There are dependencies among rows and column during factorization

Matrix Multiplication Cholesky factorization Triangular Solve (TRSM)



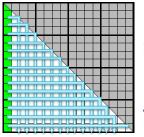
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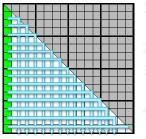
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Matrix Multiplication Cholesky factorization Triangular Solve (TRSM)

# 2D Cholesky factorization with overlapping

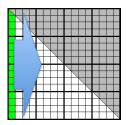
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#### 1. Factorize the $1^{st}$ block-column

- 2. Broadcast factorized column
- 3. Update & factorize **only** the 2<sup>nd</sup> block-column
- 4. Overlap
  - broadcast of the 2<sup>nd</sup> block-column
  - update of the rest trailing matrix (using 1<sup>st</sup> block-column)

Matrix Multiplication Cholesky factorization Triangular Solve (TRSM)

# 2D Cholesky factorization with overlapping



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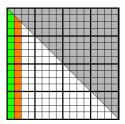
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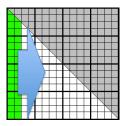
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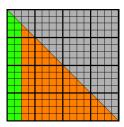
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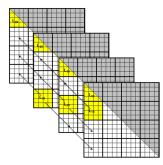


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Matrix Multiplication Cholesky factorization Triangular Solve (TRSM)

2.5D Cholesky factorization [McColl and Tiskin 99], [Solomonik and Demmel 11]

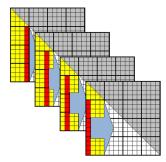
Employ two levels of blocking: "Fat panels" and "blocks"



- 1. All layers jointly factorize a "fat" panel
- Broadcast different subpanels within each layer & update trailing matrices
- 3. All-reduce the next "fat" panel to accumulate the updates

Matrix Multiplication Cholesky factorization Triangular Solve (TRSM)

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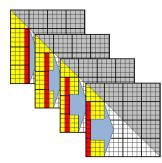


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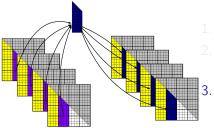
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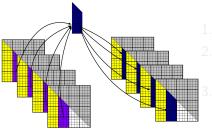


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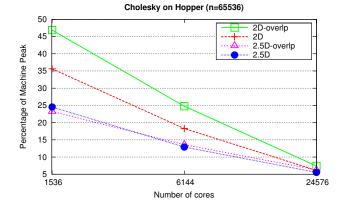
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At step 2 we can overlap computation and communication similarly to the 2D version

Matrix Multiplication Cholesky factorization Triangular Solve (TRSM)

# Performance results on Hopper (Cray XE6)

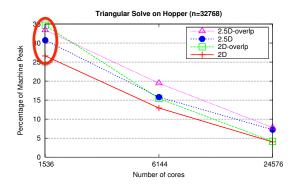


- CO helps more at the smallest scale (1,536 cores)
- Have not reached yet the cross-point of CA and 2D
- Future work: Aggregate updates to improve performance

Matrix Multiplication Cholesky factorization Triangular Solve (TRSM)

# Triangular Solve (TRSM)

- Computes X, such that  $X \cdot U = B$  with upper-triangular U
- Similar parallelization to Cholesky

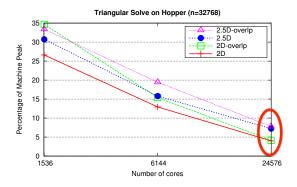


At small scale overlapping outperforms other versions

Matrix Multiplication Cholesky factorization Triangular Solve (TRSM)

# Triangular Solve (TRSM)

- Computes X, such that  $X \cdot U = B$  with upper-triangular U
- Similar parallelization to Cholesky



- At small scale overlapping outperforms other versions
- At large scale the combining optimizations is the best option

Motivation Methodology

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Motivation Methodology

### Can we explain the behavior of CO and CA?

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Effect Parameter	# messages	load balance	computation efficiency
block size 🛧	4	<b>V</b>	◆
replication <b>↑</b>	^/↓	^/↓	NA
fat panel size <b>↑</b>	<b>V</b>	→	NA

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fat panel size∱	¥	V	NA

Communication performance depends on number of processors

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- Communication performance depends on number of processors
- Given a problem instance and a machine configuration would like to predict the optimal variant

Methodology for constructing performance models

We construct detailed performance models

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  - Inputs: matrix size, # of processors, BLAS efficiency, LogGP parameters, block sizes, replication factors, fat panel sizes

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  - Estimate computation times through BLAS microbenchmarks

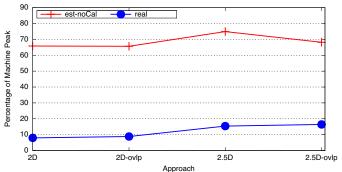
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- We track the execution flow of each algorithm and estimate completion time for encountered operation
  - Estimate computation times through BLAS microbenchmarks
  - Estimate communication times through LogGP model (collective models from [Thakur, Rabenseifner, Gropp 2005])

## Methodology for constructing performance models

- We construct detailed performance models
  - Inputs: matrix size, # of processors, BLAS efficiency, LogGP parameters, block sizes, replication factors, fat panel sizes
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- We take into account possible idle times

Motivation Methodology

#### First approach: Ignore network congestion

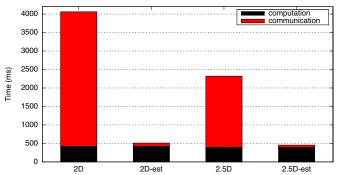


SUMMA with 24,576 cores

- We predict correctly the relative performance of the CA algorithms
- Prediction of absolute performance is inaccurate

Motivation Methodology

#### First approach: Ignore network congestion



Real and estimated times for SUMMA (24K cores, n=32,768)

- We predict accurately the computation time
- $\blacktriangleright$  We ignore congestion  $\rightarrow$  optimistic communication time

Motivation Methodology

### Quantify degradation due to congestion

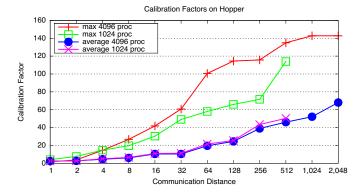
Calibration factor: <u>ideal BW</u> when several processes use the network simultaneously

### Quantify degradation due to congestion

- Calibration factor: <u>ideal BW</u> when several processes use the network simultaneously
- Extract calibration factors via microbenchmarks

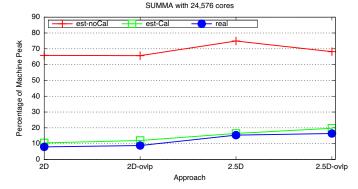
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Motivation Methodology

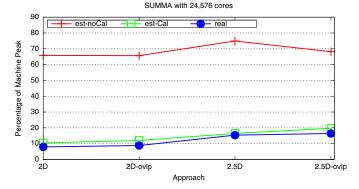
#### Including calibration factors in the models



We predict accurately the absolute performance

Motivation Methodology

### Including calibration factors in the models



- We predict accurately the absolute performance
- Similar results for the rest algorithms

### Table of contents

- Communication is Expensive
- Communication avoidance vs Overlapping
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4 Conclusions Conclusions

Conclusions

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1. Which is more important? CA or CO?

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  - ► For core counts where communication and computation are balanced CO helps more (up to 1.82× speedup)
  - ► For larger core counts CA is more beneficial (up to 2.08× speedup)

#### Conclusions

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  - We developed detailed performance models
  - They encapsulate complicated interactions between parameters
  - They predict correctly the performance

Conclusions

# Thank you!