Automatic Code Generation for High-Performance Graph Algorithms

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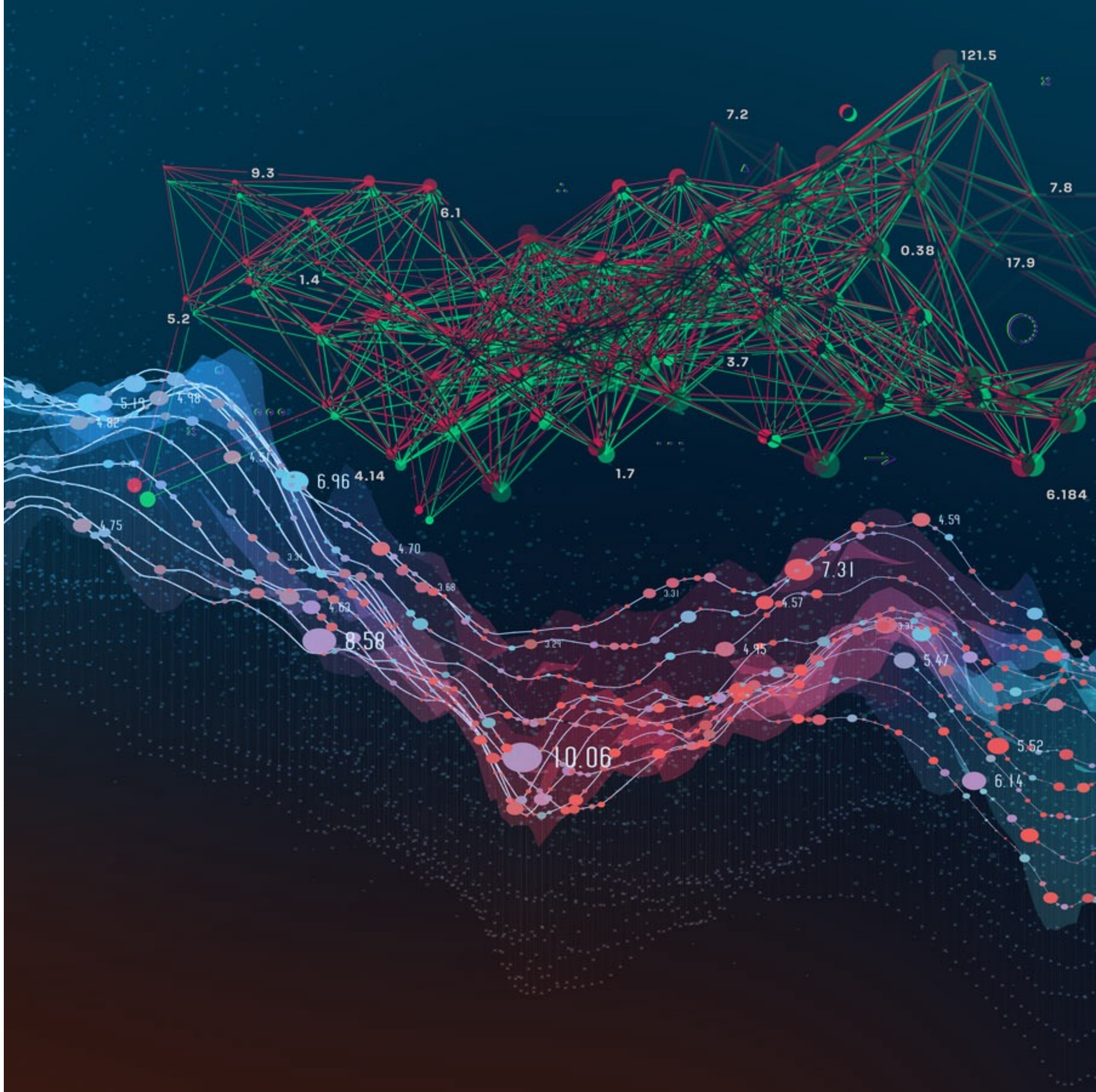
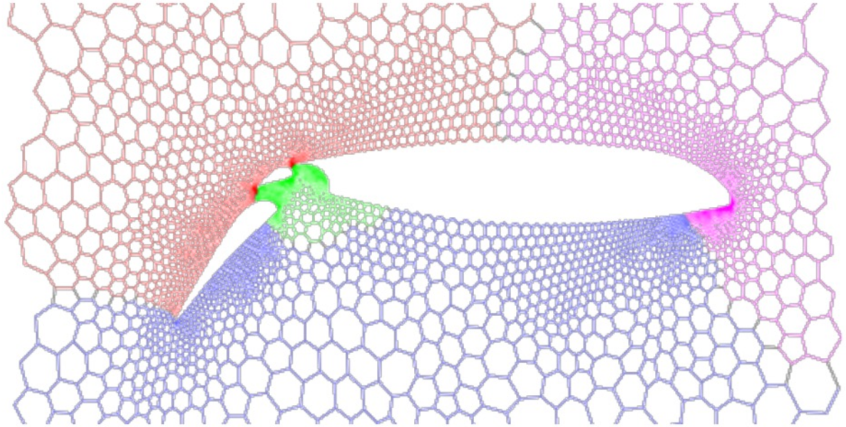


Graph Algorithms

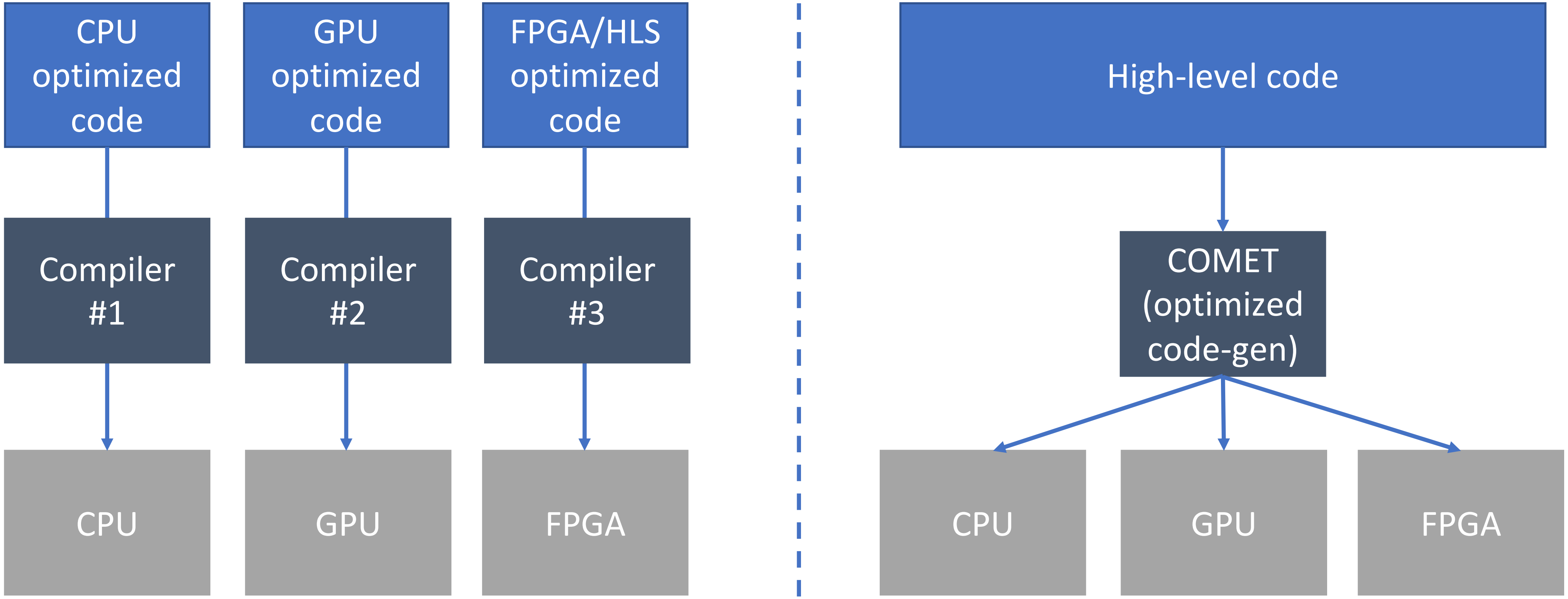
- The use of graph processing is everywhere around us!
  - Social Networks: recommendation systems
  - Travel: Shortest paths, food/hotel recommendations, etc.
  - …
  - Scientific Computing: Biology (genome assembly, human brain), Power Grid, Load Balancing.

- There are a variety of graph algorithms
  - Graph libraries exist for various targets.
  - We propose a compiler approach.



Picture Credit: Sanders and Schulz

The Compiler Approach



CPU optimized code → Compiler #1 → CPU

GPU optimized code → Compiler #2 → GPU

FPGA/HLS optimized code → Compiler #3 → FPGA

3X effort for writing libs (in most cases)

High-level code → COMET (optimized code-gen) → CPU, GPU, FPGA

Write once, run anywhere

COMET: COMpiler for Extreme Targets

- Porting graph applications to heterogeneous systems often requires porting code to different programming environments.
  - Explosion of complexity and versioning.
  - Difficult to achieve performance portability.
- For performance portability, need to identify computational patterns.
  - High-level languages allow users to express high-level computational patterns/motifs.
  - Semantics information is used for efficient code generation.
- Clear separation of responsibilities.
  - Users implement algorithms using high-productive programming environments.
  - Compiler generates efficient code for heterogeneous architectures.

The Challenge with Graph Algorithms

- Traditional architectures are mostly designed for structured data accesses (lists, stacks, etc.).
  - Graph algorithms operate on irregular sparse data.
  - The time spent in communication is high as compared to computation.
  - Conventional latency hiding techniques do not provide much benefit.
- Challenge to program efficient graph algorithms
  - Random access patterns provides poor locality in cache, and hence lot of misses.
  - Parallelization is difficult.
- Optimizations if performed severely limit portability of graph algorithms to new architectures.
  - Compilers can help, but we also need a new way of doing graph algorithms.

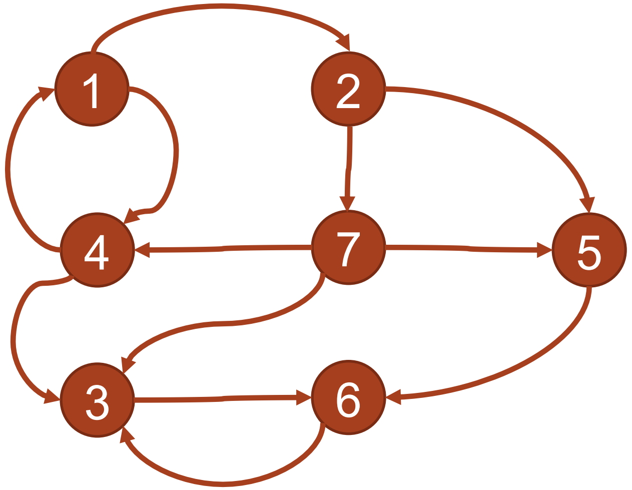
Graph Algorithms in Linear Algebra

- Linear algebra (LA) provide an elegant, concise, intuitive, and portable programming abstraction for implementing graph algorithms.
    - The algorithmic complexity of LA-based implementations is close to the complexity of the node- or edge-traversal-based implementations.
- Linear algebra operators have been extensively studied and optimized for a variety of architectures and domain problems
    - Many algorithmic implementations of operators and methods
    - Many LA accelerators exists (e.g., Tensor cores)
    - Good support in many architectures (e.g., AVX)
    - LA operators represent basic computational blocks in emerging architecture

LA-based Graph Processing

- A graph as a sparse adjacency matrix.
- Sparse matrix/vector operations can be used to express graph algorithms.

	1		1			
				1		1
					1	
1		1				
					1	
		1				
		1	1	1		



LA-based Graph Processing

- A graph as a sparse adjacency matrix.
- Sparse matrix/vector operations can be used to express graph algorithms.
    - Find vertices that are one hop away from a source vertex: fA

Only operations are performed where non-zero elements exist

A

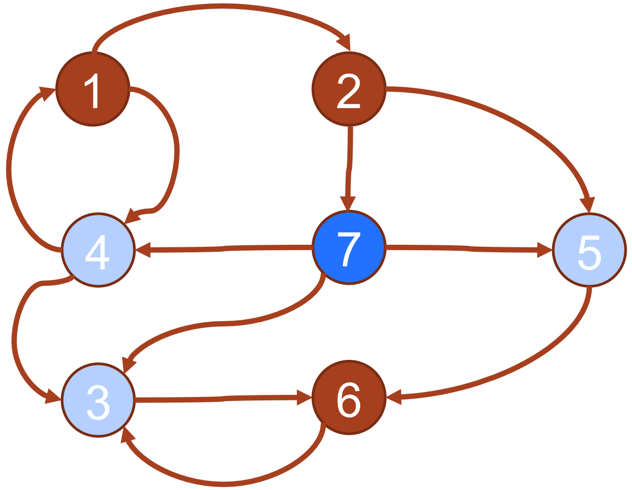
	1		1			
				1		1
					1	
1		1				
					1	
		1				
		1	1	1		

Frontier, f

						1

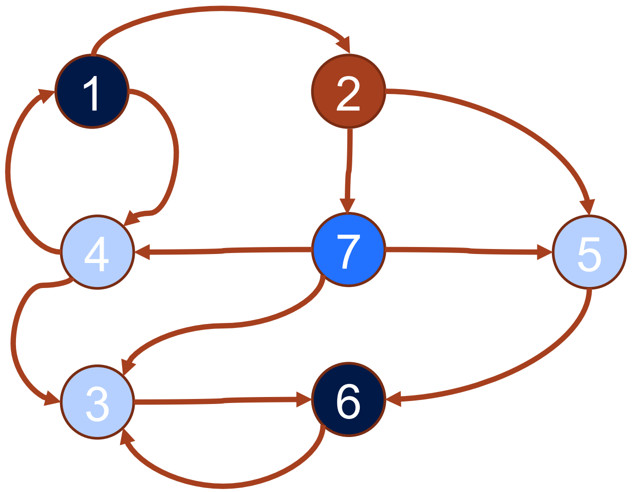
		1	1	1		

fA



LA-based Graph Processing

- A graph as a sparse adjacency matrix.
- Sparse matrix/vector operations can be used to express graph algorithms.
  - Find vertices that are k hops away from a source vertex: fA^k



A

	1		1			
				1		1
					1	
1		1				
					1	
		1				
		1	1	1		

	1		1			
				1		1
					1	
1		1				
					1	
		1				
		1	1	1		

						1

Frontier, f

		1	1	1		

fA

1		1			2	

fA^2

Semirings

- A semiring is an algebraic structure that allows us to perform special operations beyond addition and multiplication to elements in a generic matrix multiplication operation.

Any-pair semiring for traversal. Operates on binary values (structure).

Frontier f

			1		1	

A

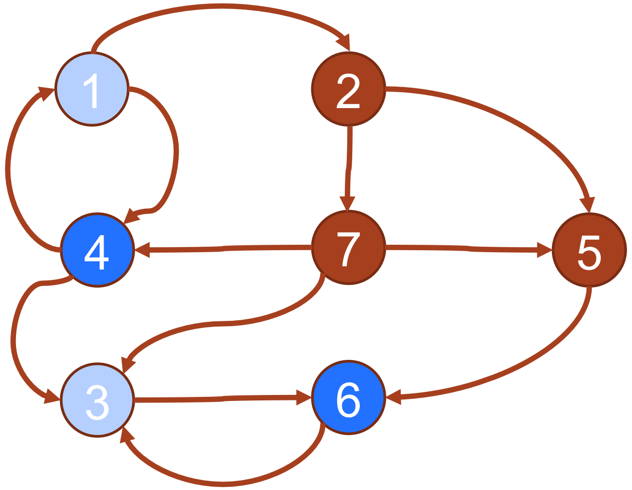
	1		1			
				1		1
					1	
1		1				
					1	
		1				
		1	1	1		

Any (pair(1,1), pair(1,1))

1		1				

$w = f@(any, pair)A$

$f@(+,\times)\ A$



Semirings

- A semiring is an algebraic structure that allows us to perform special operations beyond addition and multiplication to elements in a generic matrix multiplication operation.

Plus-times semiring for traversal. Operates on natural numbers.

A

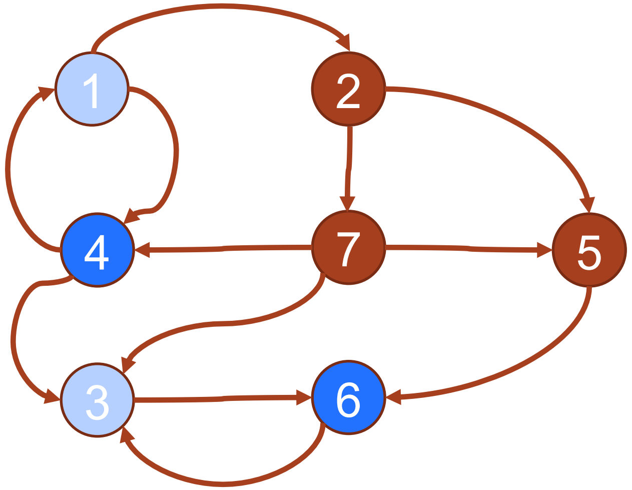
	1		1			
				1		1
					1	
1		1				
					1	
		1				
		1	1	1		

Frontier f

			1		1	

1		2				

$w = f@(+,\times)\,A$



Semirings

- A semiring is an algebraic structure that allows us to perform special operations beyond addition and multiplication to elements in a generic matrix multiplication operation.

Min-Plus semiring for finding shortest path. Operates on +Real numbers.

Frontier f

			0.5		0.6	

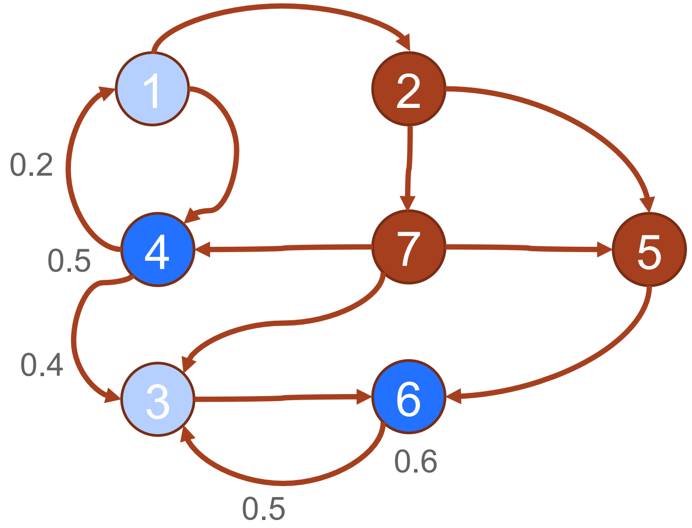
A

	1		1			
				1		1
					1	
0.2		0.4				
					1	
		0.5				
		1	1	1		

Min (0.5+0.4, 0.6+0.5)

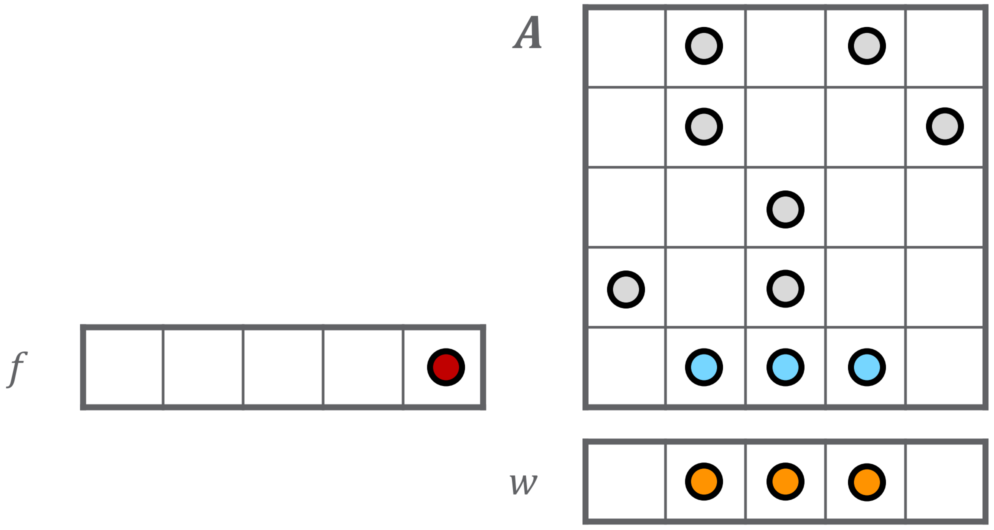
0.7		0.9				

$w = f@(min, +)A$



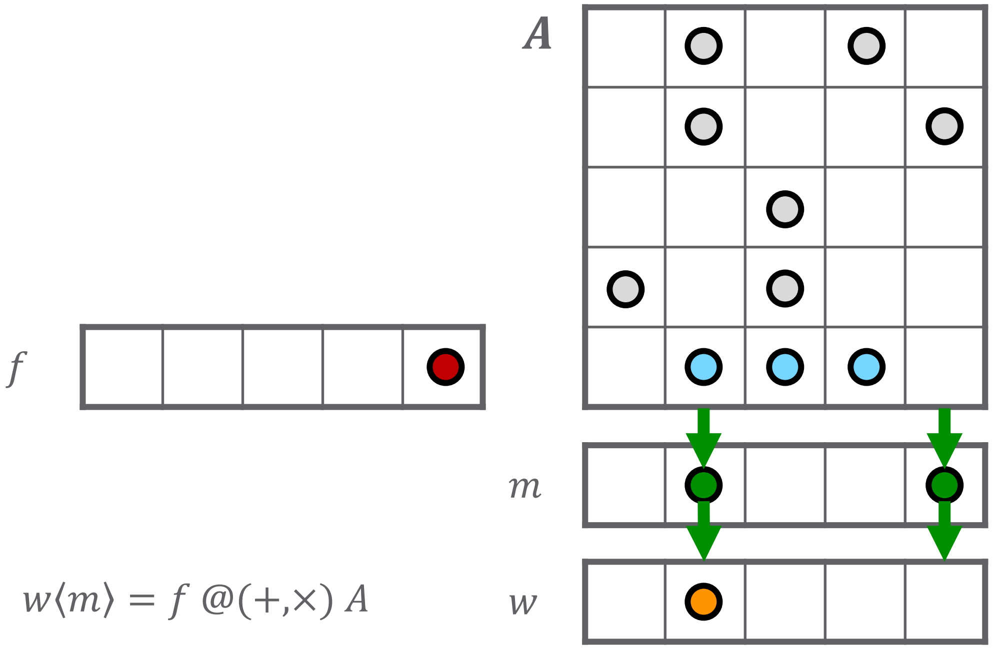
Masking

- Prevent redundant computations (traversal: already visited vertices)
- Reduce the scope of an operation to be performed
  - A mask indicates the locations where the operation should be performed



$w = f\ @(+,\times)\ A$

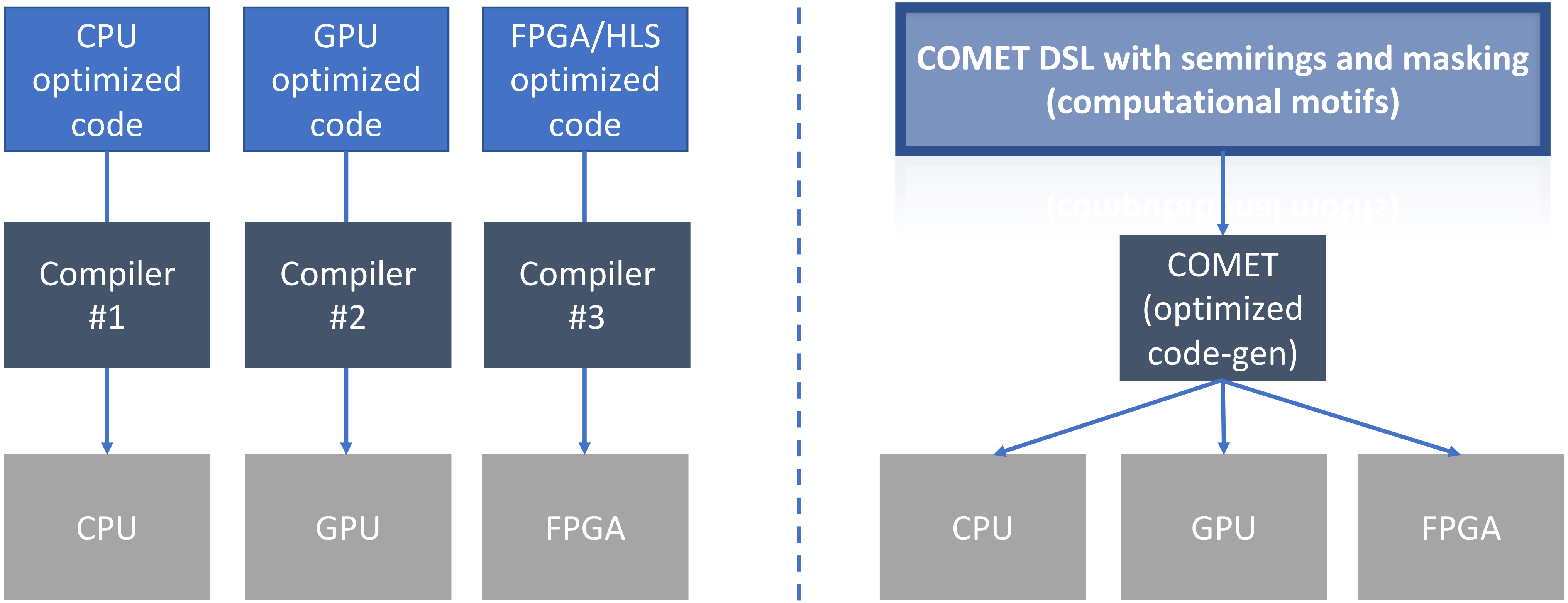
without a mask



$w\langle m\rangle = f\ @(+,\times)\ A$

with a mask

A DSL for Graph Algorithms using Linear Algebra



CPU optimized code

GPU optimized code

FPGA/HLS optimized code

Compiler #1

Compiler #2

Compiler #3

CPU

GPU

FPGA

3X effort for writing libs (in most cases)

COMET DSL with semirings and masking (computational motifs)

COMET (optimized code-gen)

CPU

GPU

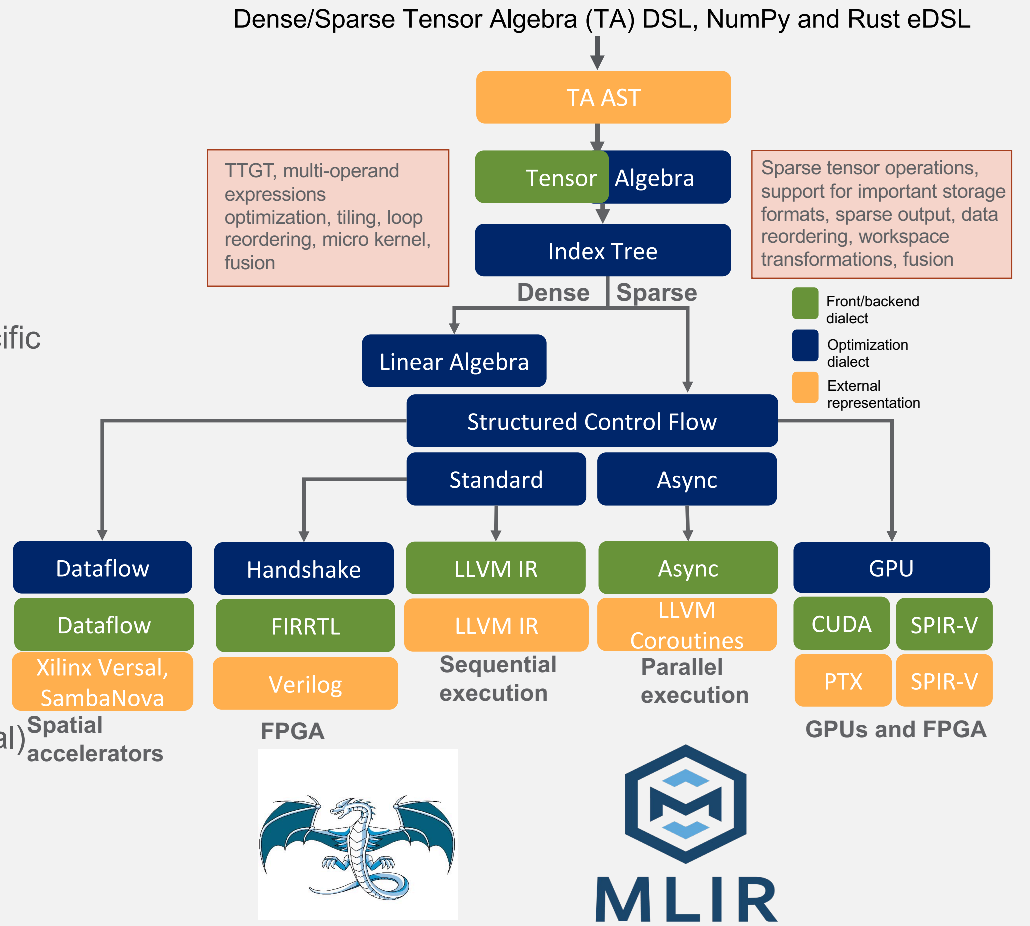
FPGA

Write once, run anywhere

COMET: Domain Specific Compilation in Multi-level IR

- COMET is a compiler infrastructure that focuses on computational chemistry and graph analytics application domain
- COMET supported frontends
  - COMET Domain specific language that follows Einstein notation
  - NumPy einsum to evaluates the Einstein summation
  - Rust eDSL
- COMET compiler infrastructure
  - Enable from high-level, domain-specific and low-level, architecture-specific compiler optimizations
  - **Tensor algebra dialect** in the MLIR infrastructure
  - **Multi-level** code optimizations, including domain-specific and architecture specific
  - **Abstraction** for dense/sparse storage formats
    - ✓ A set of per-dimension attributes to specify sparsity properties of tensors
    - ✓ Attributes enables support for **a wide range of sparse storage formats**
  - Data layout optimizations to enhance **data locality**
  - Support for **sparse output** for sparse-sparse computation (e.g., SpGEMM)
  - Support for **semiring** operations to represent graph algorithms
  - **Kernel Fusion** to avoid temporaries and redundant computation
  - Automatic code generation for **sequential** and **parallel** execution
  - **FPGA** code generation via SPIRV binary
  - Interface with **emerging dataflow architectures** (SambaNova and Xilinx Versal)
- COMET runtime
  - **Input-dependent optimization** to increase data locality and load balancing
  - Read input matrices and tensors, convert it into internal storage format

$$C_{ijkl} = \sum_{mn} A_{imkn} \cdot B_{jnlm}$$



Multi-Level Intermediate Representation (MLIR)

A collection of modular and reusable software components that enables the progressive lowering of high-level operations, to efficiently target hardware in a common way

New compiler infrastructure

Part of LLVM project

https://github.com/llvm/llvm-project

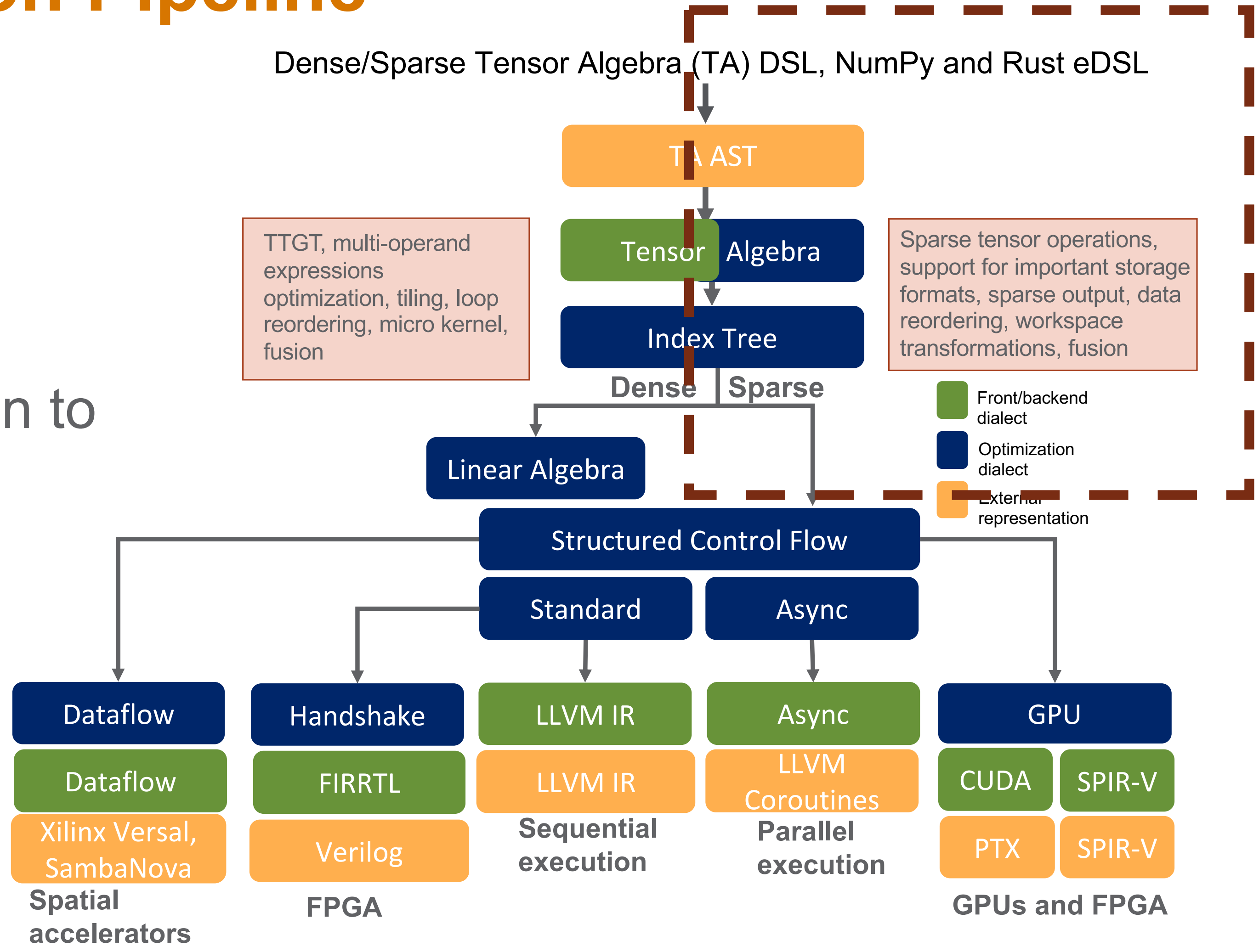
Sparse Computations

- Sparse kernels are widely used in many applications, e.g., scientific computing, machine learning, and data analytics
- Sparse computations uses sparse storage formats:
  - To reduce storage requirements by storing only nonzero elements
  - To reduce computational requirements by skipping redundant computation
- Challe
  - Dif
  - Lack of temporal locality due to irregular accesses
  - Lack of spatial locality, limited data reuse
- Sparse libraries solve some of the issues above but …
  - Limited support for combination of sparse storage formats, various tensor expressions, and heterogeneous target architectures

Sparse Compilers simplifies development of sparse kernels by automatically generating code based on tensor “***sparsity”*** property

Sparse Compilation Pipeline[1,2]

- Internal sparse tensor storage format
- Sparse data type
- An attribute per tensor dimension to support sparse tensor storage format
- Automatic code generation for sparse tensor operations
- Support for sparse output
- Input-dependent optimization
  - Data reordering to enhance data locality



Dense/Sparse Tensor Algebra (TA) DSL, NumPy and Rust eDSL

TA AST

Tensor Algebra

Index Tree

Dense | Sparse

TTGT, multi-operand expressions optimization, tiling, loop reordering, micro kernel, fusion

Sparse tensor operations, support for important storage formats, sparse output, data reordering, workspace transformations, fusion

🟩 Front/backend dialect

🟦 Optimization dialect

🟧 External representation

Linear Algebra

Structured Control Flow

Standard

Async

Dataflow → Dataflow → Xilinx Versal, SambaNova — **Spatial accelerators**

Handshake → FIRRTL → Verilog — **FPGA**

LLVM IR → LLVM IR — **Sequential execution**

Async → LLVM Coroutines — **Parallel execution**

GPU → CUDA, SPIR-V → PTX, SPIR-V — **GPUs and FPGA**

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[1] Ruiqin Tian, Luanzheng Guo, Jiajia Li, Bin Ren, Gokcen Kestor. “A High Performance Sparse Tensor Algebra Compiler in MLIR”. *LLVM-HPC*, 2021.
[2] Sparse tensor algebra optimizations in MLIR. Tian R., L. Guo, and G. Kestor. 2021 LLVM DEVELOPERS' MEETING. November 2021.

Support for Sparse Outputs

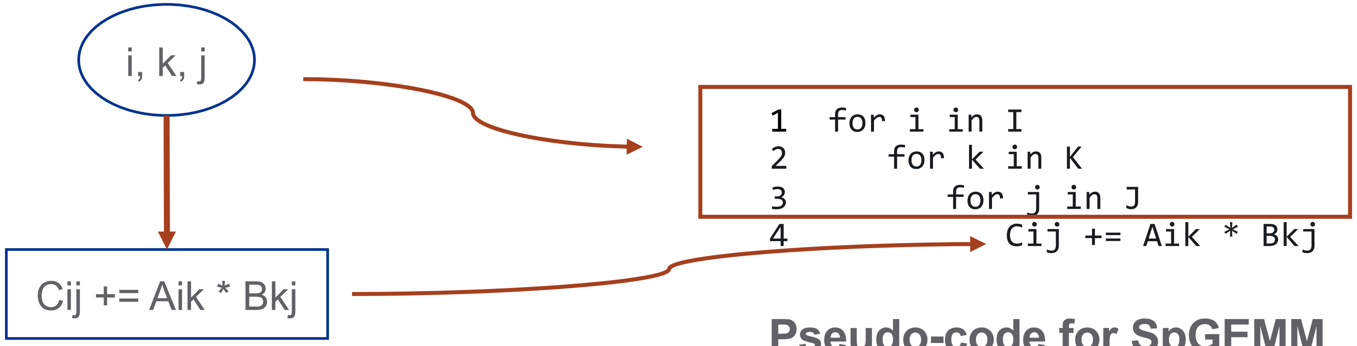
- Storing output tensor in a sparse format introduces expensive insertions and accesses to sparse input tensors, which has large time complexity
- We introduced a **temporary dense data structure** (called workspaces[1]) to store the value in the sparse dimension in sparse kernels to improve **data locality** of sparse kernels while producing **sparse output**
- This approach brings the following advantages:
  - Significantly improves performance of sparse kernels through efficient dense data structures accesses.
  - Reduces memory footprint
  - Avoids “densifying” issue in the compound expressions

[1] Tensor Algebra Compilation with Workspaces. Fredrik Kjolstad, and et al., IEEE/ACM International Symposium on Code Generation and Optimization, 2019

Index tree Intermediate Representation (IR)

- We introduced ***Index Tree*** intermediate representation in the COMET compiler
  - Index Tree is a high-level intermediate representation for a tensor expression
  - Consists of two types of nodes
    - ✓ **Index nodes:**
      - Contain one or more indices to represent (nested) loops
      - Each index represent a level of loop
    - ✓ **Compute nodes:**
      - Contain compute statements

$$Cij = \sum_{k} Aik \ * Bkj$$



```
for i in I
   for k in K
      for j in J
         Cij += Aik * Bkj
```

Index tree for SpGEMM

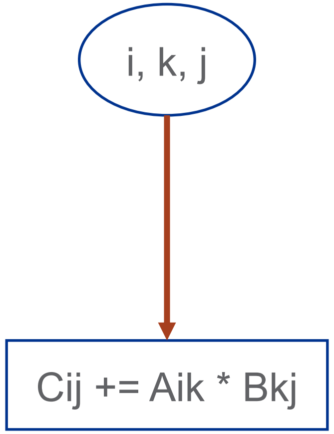
Pseudo-code for SpGEMM

Workspace Transformation

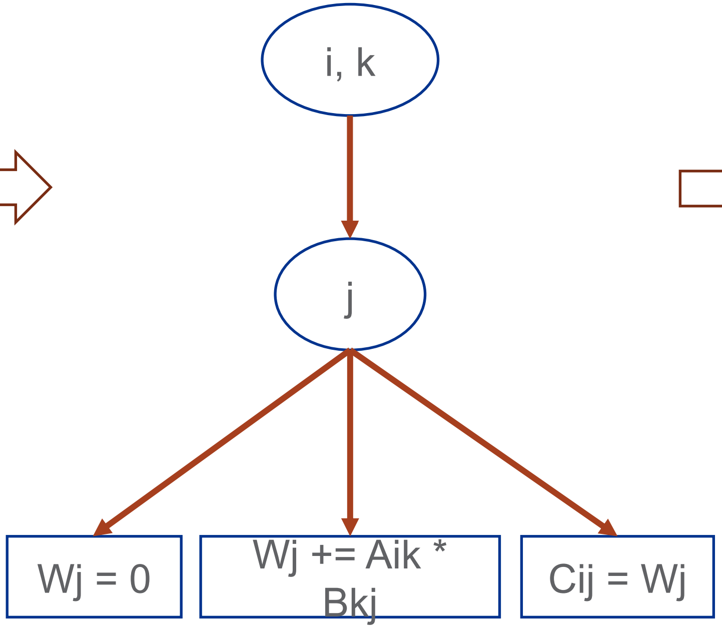
- We perform compiler transformation in the index tree representation of a tensor expression
  - Benefits
    - ✓ Reduces expensive insertions/ accesses to sparse tensors
      - Dense data structure has better locality
      - Generates “for” loops instead of “while” loops
      - Utilize the existing for loop optimizations
  - How?
    - ✓ Identify the index that needs workspace
      - Store the value in the dimension into workspace (i.e., dense low dimensional data structure)
    - ✓ Check output tensor (lhs) , if it contains sparse dimension
      - e.g., SpGEMM in CSR, dimension j is sparse in C. Then the original “Cij=Aik*Bkj” will be transformed into “Wj = 0; Wj += Aik*Bkj; Cij = Wj; ” in each iteration of i
    - ✓ Check input tensors (rhs), if one dimension in both two input tensors are sparse
      - e.g., pure sparse elementwise multiplication, Cij=Aij*Bij, all matrices are in CSR. In this case, dimension j is sparse in A and B. then the original “Cij=Aij*Bij” will be converted into “Wj = 0;Wj = Aij; Cij = Wj*Bij;” in each iteration of i

What is the algorithm?

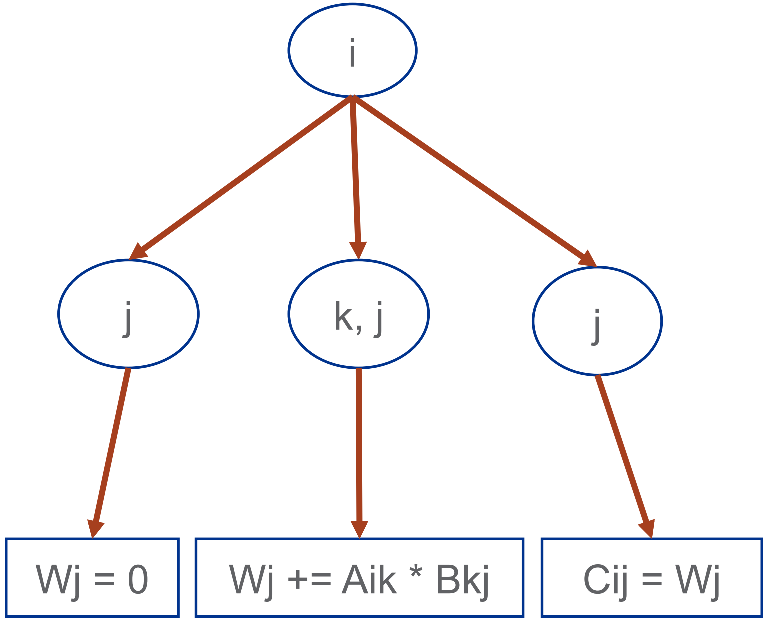
Transformation in Index Tree



Index tree for SpGEMM

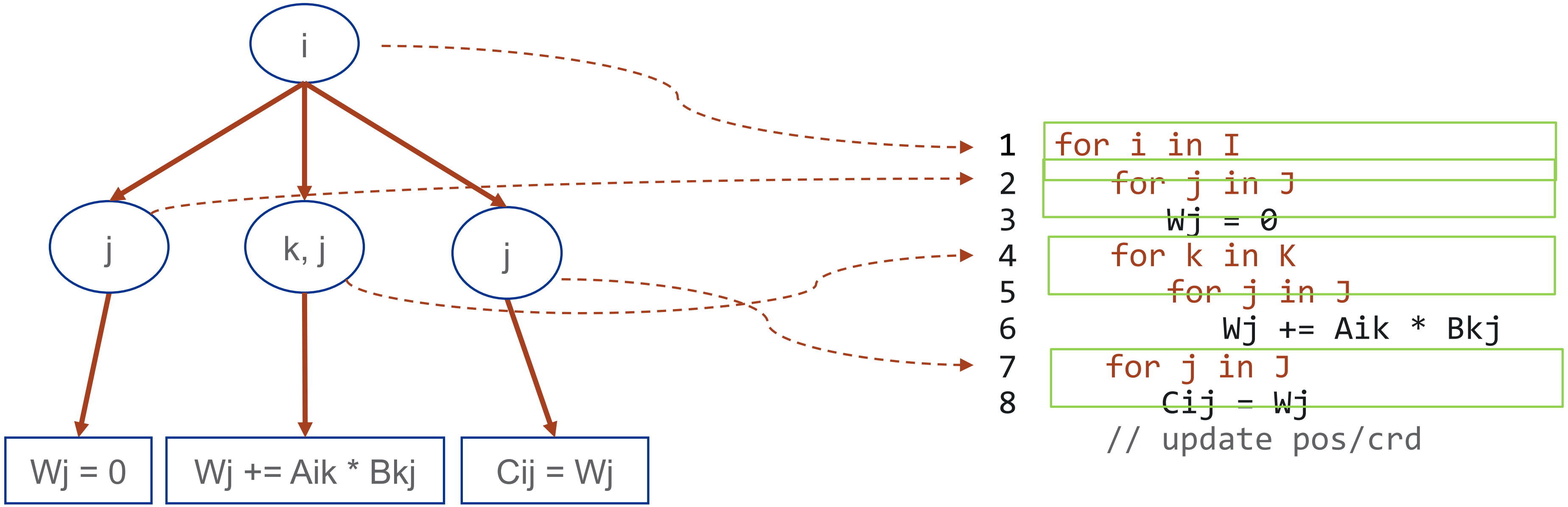


Index tree for SpGEMM with workspace



Eliminate loop invariant redundancy

Code Generation from Index Tree IR Operations



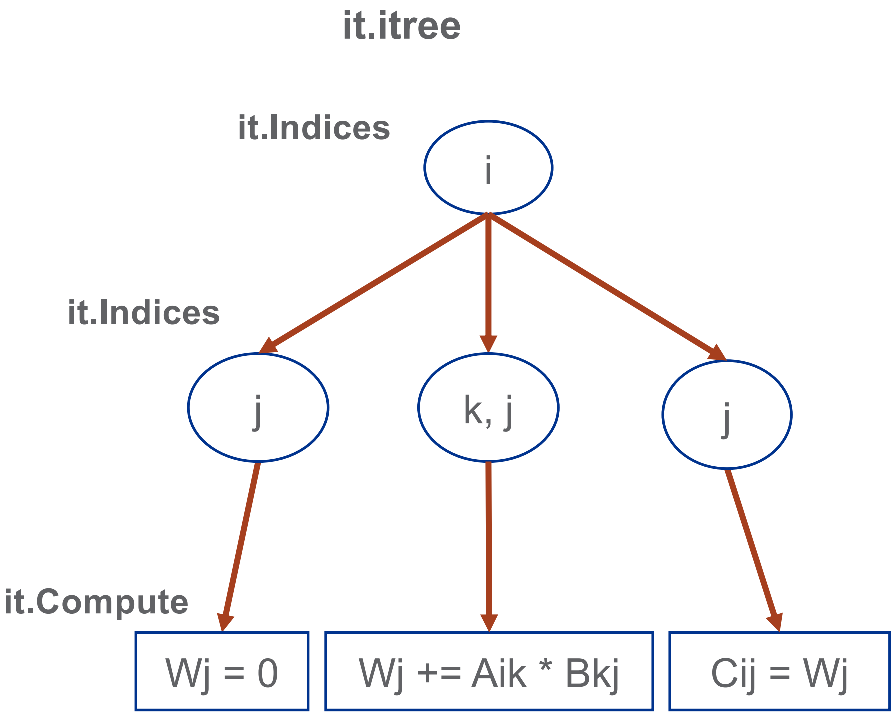
```
for i in I
  for j in J
    Wj = 0
  for k in K
    for j in J
      Wj += Aik * Bkj
  for j in J
    Cij = Wj
  // update pos/crd
```

Index tree for SpGEMM

Pseudo-code for SpGEMM with workspace

Index Tree IR Operations

- Three types of index tree IR operations
  - **it.itree**: the identifier of the index tree op in IT IR
  - **it.Indices**: represent the information in Index Node in index tree
  - **it.Compute**: represent the information in Compute Node in index tree



Index tree example

```
%96 = it.Compute (%cst_40, %95) {…} : …-> (i64)
%97 = it.Indices (%96) {indices = [2]} : (i64) -> i64
%98 = it.Compute (%34, %68, %95) {semiring="plus-times"} …: -> (i64)
%99 = it.Indices (%98) {indices = [1, 2]} : (i64) -> i64
%100 = it.Compute (%95, %93) {…} -> (i64)
%101 = it.Indices (%100) {indices = [2]}
%102 = it.Indices (%97, %99, %101) {indices = [0]}
%103 = it.itree (%102) : (i64) -> i64
```

Corresponding index tree IR

Generated Index Tree IR Operations Example

```
def main() {
    #IndexLabel Declarations
    IndexLabel [i] = [?];
    IndexLabel [j] = [?];
    IndexLabel [k] = [?];

    #Tensor Declarations
    Tensor<double> A([i, k], {CSR});
    Tensor<double> B([k, j], {CSR});
    Tensor<double> C([i, j], {CSR});

    #Tensor Data Initialization
    A[i, k] = comet_read(0);
    B[k, j] = comet_read(1);
    C[i, j] = 0.0;

    #Tensor Contraction
    C[i, j] = A[i, k] @(+,*) B[k, j];
}
```

SpGEMM DSL

```
%96 = it.Compute (%cst_40, %95) {…} : …-> (i64)
%97 = it.Indices (%96) {indices = [2]} : (i64) -> i64
%98 = it.Compute (%34, %68, %95) {semiring=“plus-times”} …: -> (i64)
%99 = it.Indices (%98) {indices = [1, 2]} : (i64) -> i64
%100 = it.Compute (%95, %93) {…} -> (i64)
%101 = it.Indices (%100) {indices = [2]}
%102 = it.Indices (%97, %99, %101) {indices = [0]}
%103 = it.itree (%102) : (i64) -> i64
```

SpGEMM Index Tree IR Ops

```
for i in I
  for j in J
    Wj = 0
  for k in K
    for j in J
      Wj += Aik * Bkj
  for j in J
    Cij = Wj
  // update pos/crd
```

Pseudo-code for SpGEMM with workspace

The semiring attribute influences how this code is generated.

Some semiring examples in DSL

```
def main() {
    #IndexLabel Declarations
    IndexLabel [a] = [?];
    IndexLabel [b] = [?];
    IndexLabel [c] = [?];

    #Tensor Declarations
    Tensor<double> A([a, b], {CSR});
    Tensor<double> B([b, c], {CSR});
    Tensor<double> C([a, c], {CSR});

    #Tensor Data Initialization
    A[a, b] = comet_read(0);
    B[b, c] = comet_read(1);

    #PlusTimes semiring
    C[a, c] = A[a, b] @(+,*) B[b, c];
}
```

```
def main() {
    #IndexLabel Declarations
    IndexLabel [a] = [?];
    IndexLabel [b] = [?];


    #Tensor Declarations
    Tensor<double> A([a, b], {CSR});
    Tensor<double> B([a, b], {CSR});

    #Tensor Data Initialization
    A[a, b] = comet_read(0);
    B[a, b] = comet_read(1);


    #Min monoid
    C[a, b] = A[a, b] @(min) B[a, b];
}
```

Semiring Operations in COMET

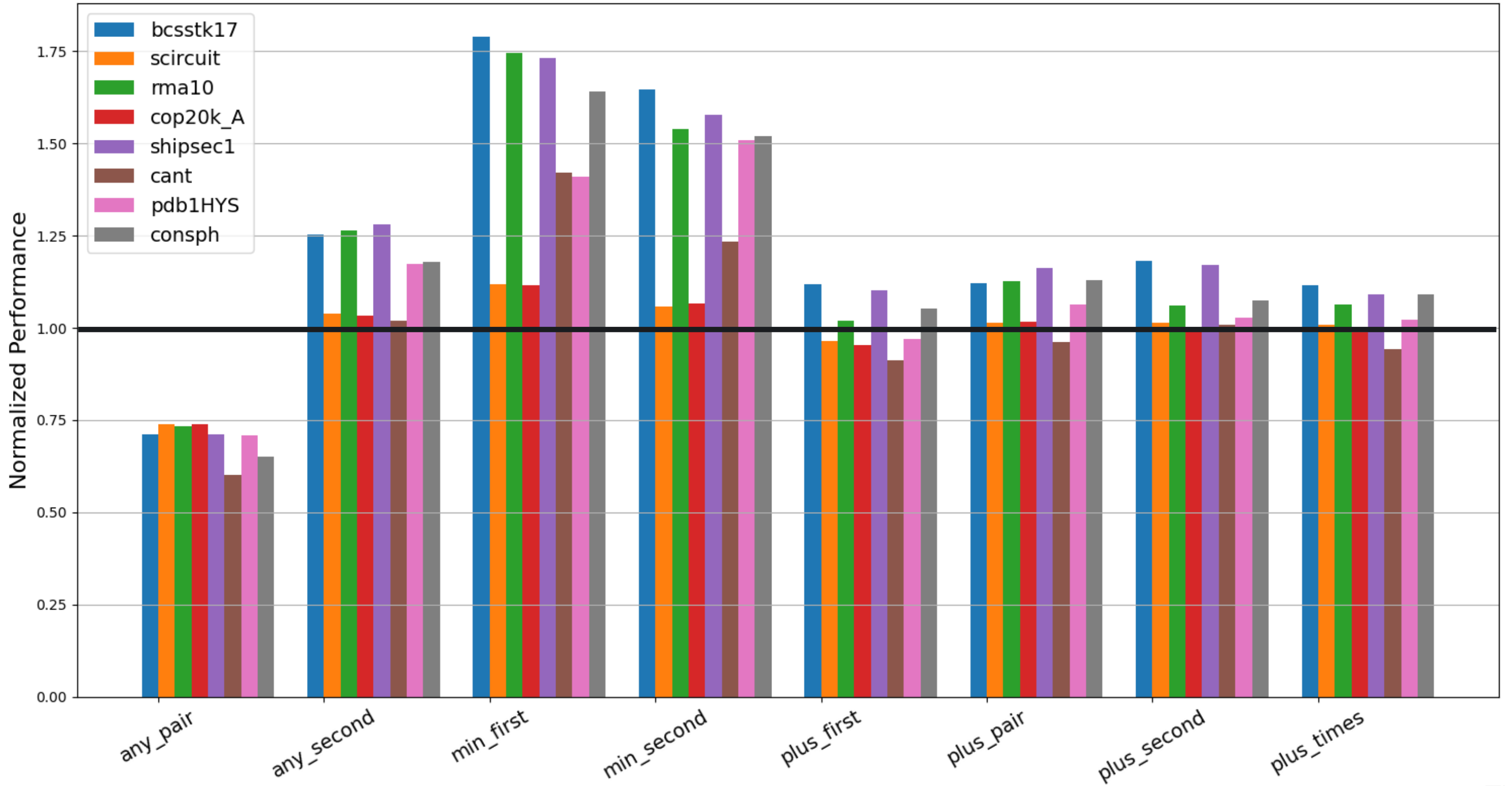
Semirings	Operation	Explanation
Lor-land	s(|, &)	‘lor’ means logical OR; ‘land’ means logical AND.
Min-first	s(min, first)	‘min’ means the minimal value; ‘first’ means first(x, y) = x: output the value of the first in the pair.
Plus-times	s(+,x)	‘+’ means addition; ‘x’ means multiplication.
Any-pair	s(any, pair)	‘any’ means “if there is any; if yes return true”. ‘pair’ means pair(x, y) = 1: x and y both have defined value at this intersection.
Min-plus	s(min, +)	‘min’ means the minimal value; ‘+’ means addition.
Plus-pair	s(+, pair)	‘+’ means addition; ‘pair’ means pair(x, y) = 1: x and y both have defined value at this intersection.
Min-second	s(min, second)	‘min’ means the minimal value; ‘second’ means second(x, y) = x: output the value of the second in the pair.
Plus-second	s(+, second)	‘+’ means addition; ‘second’ means second(x, y) = x: output the value of the second in the pair.
Plus-first	s(+, first)	‘+’ means addition; ‘first’ means first(x, y) = x: output the value of the first in the pair.

Semiring Operations per application

	Semirings	Operation	Description
BFS	Lor-land	s(|, &)	Compute traversal level for each vertex
	Min-first	s(min, first)	Compute parent for each vertex
	Plus-times	s(+,x)	Number of paths
	Any-pair	s(any, pair)	Reachability
	Min-plus	s(min, +)	Shortest path
SSSP	Min-plus	s(min, +)	Shortest path without mask (Bellman-Ford Algorithm)
TC	Plus-pair	s(+, pair)	Number of triangles
CC	Min-second	s(min, second)	Hooking and shortcutting
PR	Plus-second	s(+, second)	Outbound PageRank score
BC	Plus-first	s(+, first)	Accumulate path count

Semiring Performance (unjumbled)

- A method returns a matrix in an *unjumbled* state, with indices sorted
  - if the matrix will be immediately exported in unjumbled form, or
  - if the matrix is provided as input to a method that requires it to not be jumbled

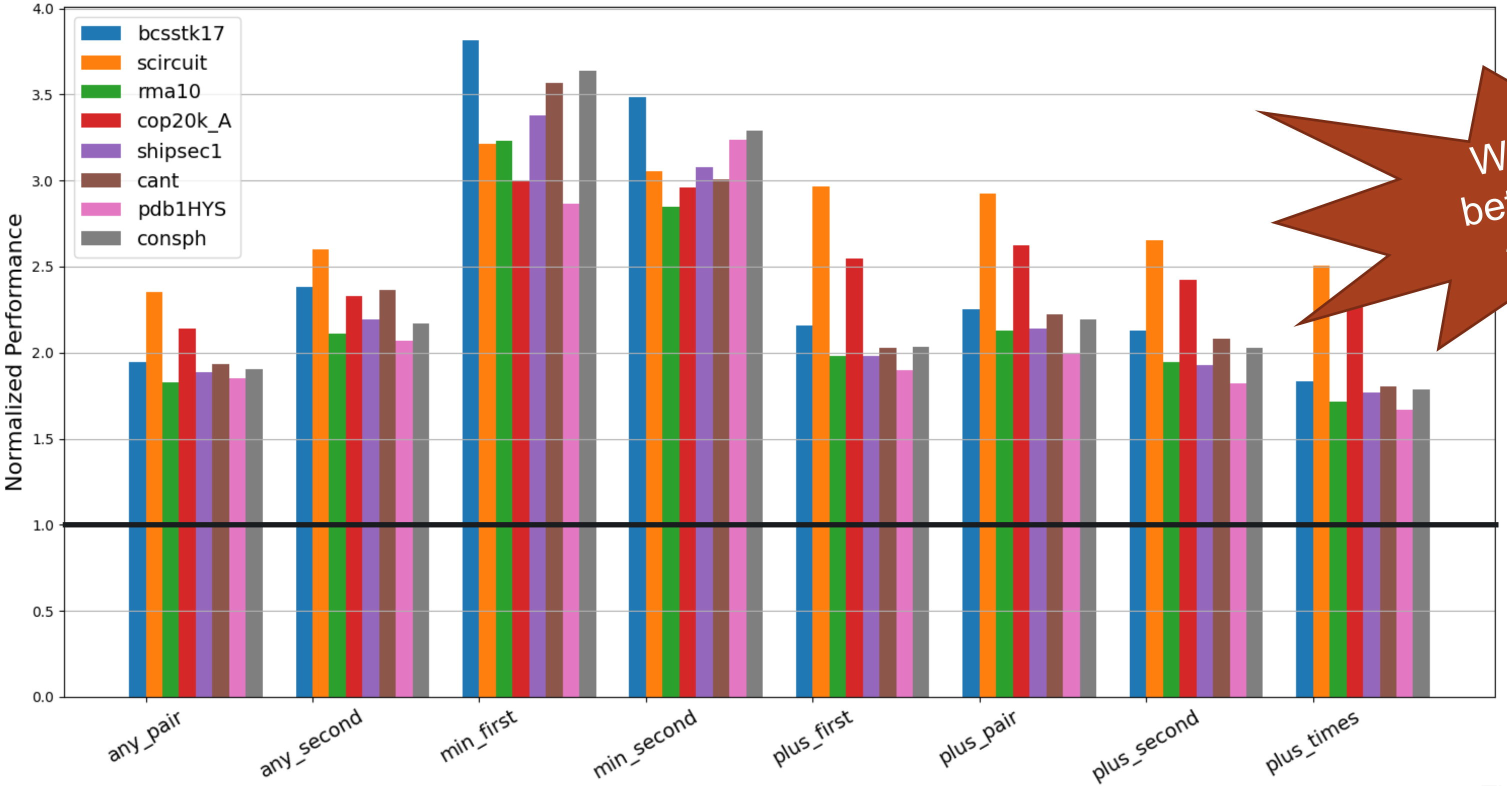


Performance comparison wrt LAGraph[1]

[1] Tim Mattson and others. “LAGraph: A Community Effort to Collect Graph Algorithms Built on Top of the GraphBLAS”, IEEE International Parallel and Distributed Processing Symposium Workshops (IPDPSW), 2019.

Semiring Performance (jumbled)

- A method returns a matrix in a *jumbled* state, with indices out of order
  - If some methods can tolerate jumbled matrices on input, the sorting of the indices is left pending

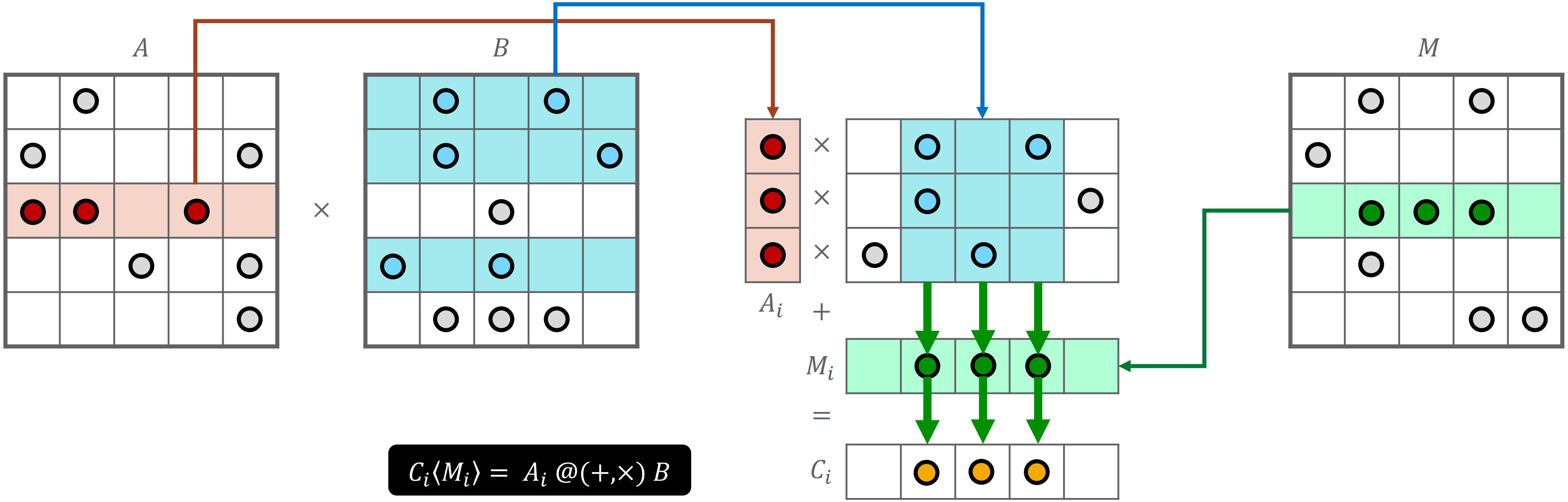


We need a better sorting algorithm

Performance comparison wrt LAGraph

Push-Based Masking

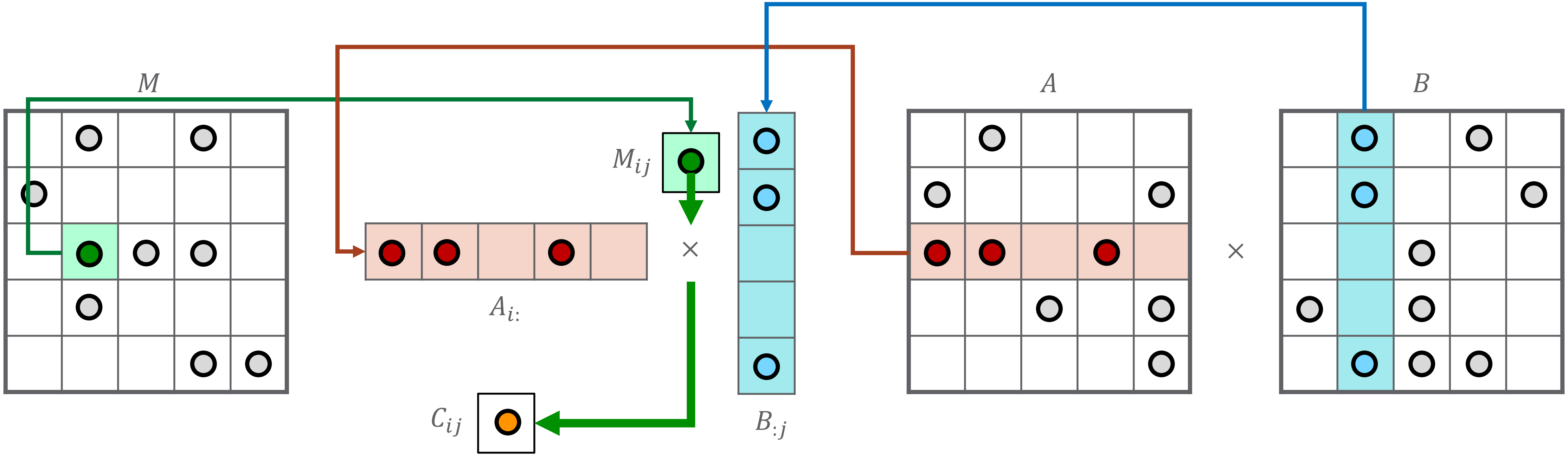
- Example of SpGEMM: $C\langle M\rangle = A\ @(+,\times)\ B$
- Driven by rows of A
- Do linear combination



$C_i\langle M_i\rangle = A_i\ @(+,\times)\ B$

Pull-Based Masking

- Example of SpGEMM: $C\langle M\rangle = A\ @(+,\times)\ B$
- Driven by non-zero elements of M
- Do dot product, and B is in CSC format



$$C_{ij}\langle M_{ij}\rangle = A_{i:}\ @(+,\times) B_{:j}$$

We plan to have pull-based masking in the future

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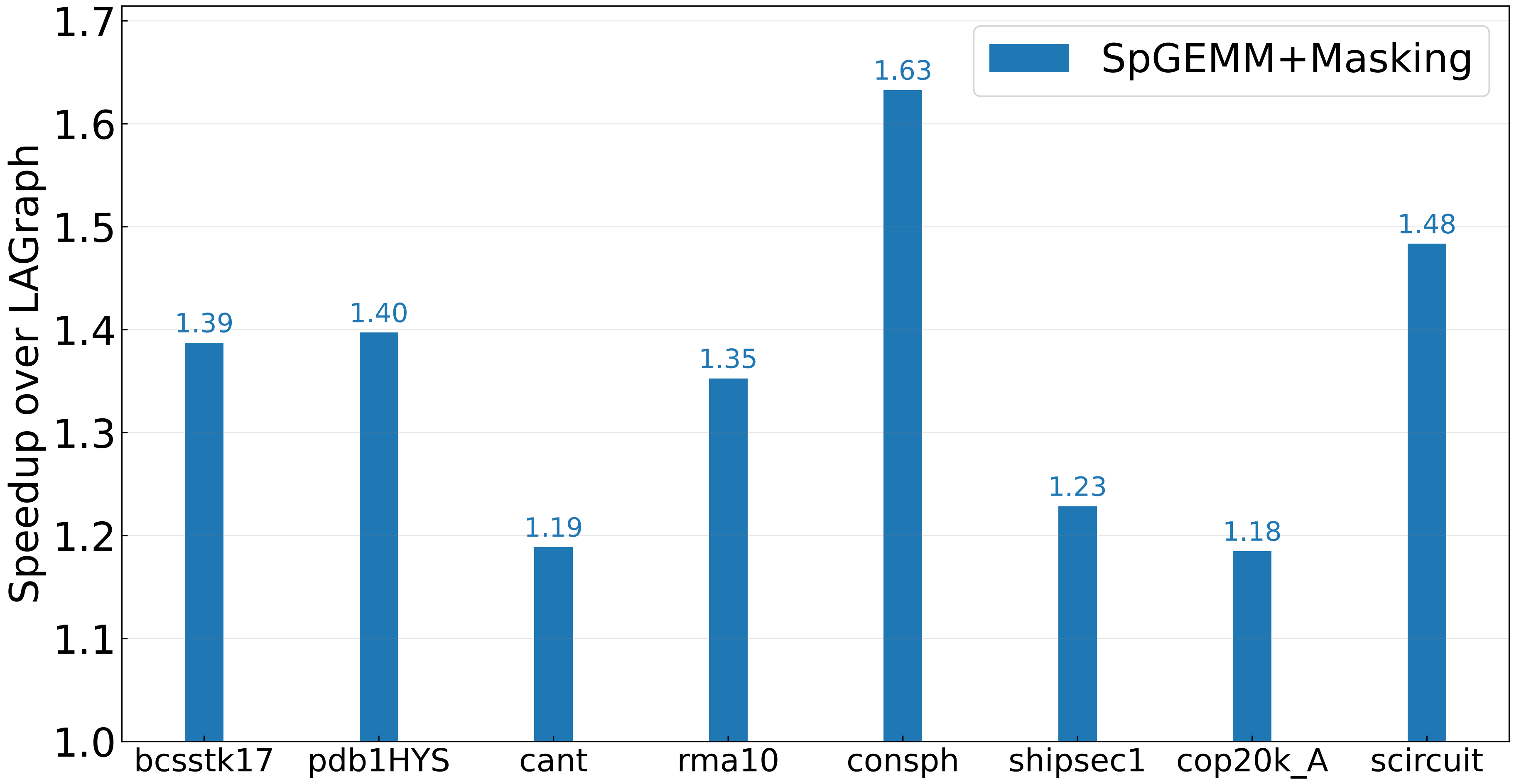
Results: Masking



Triangle Counting in COMET

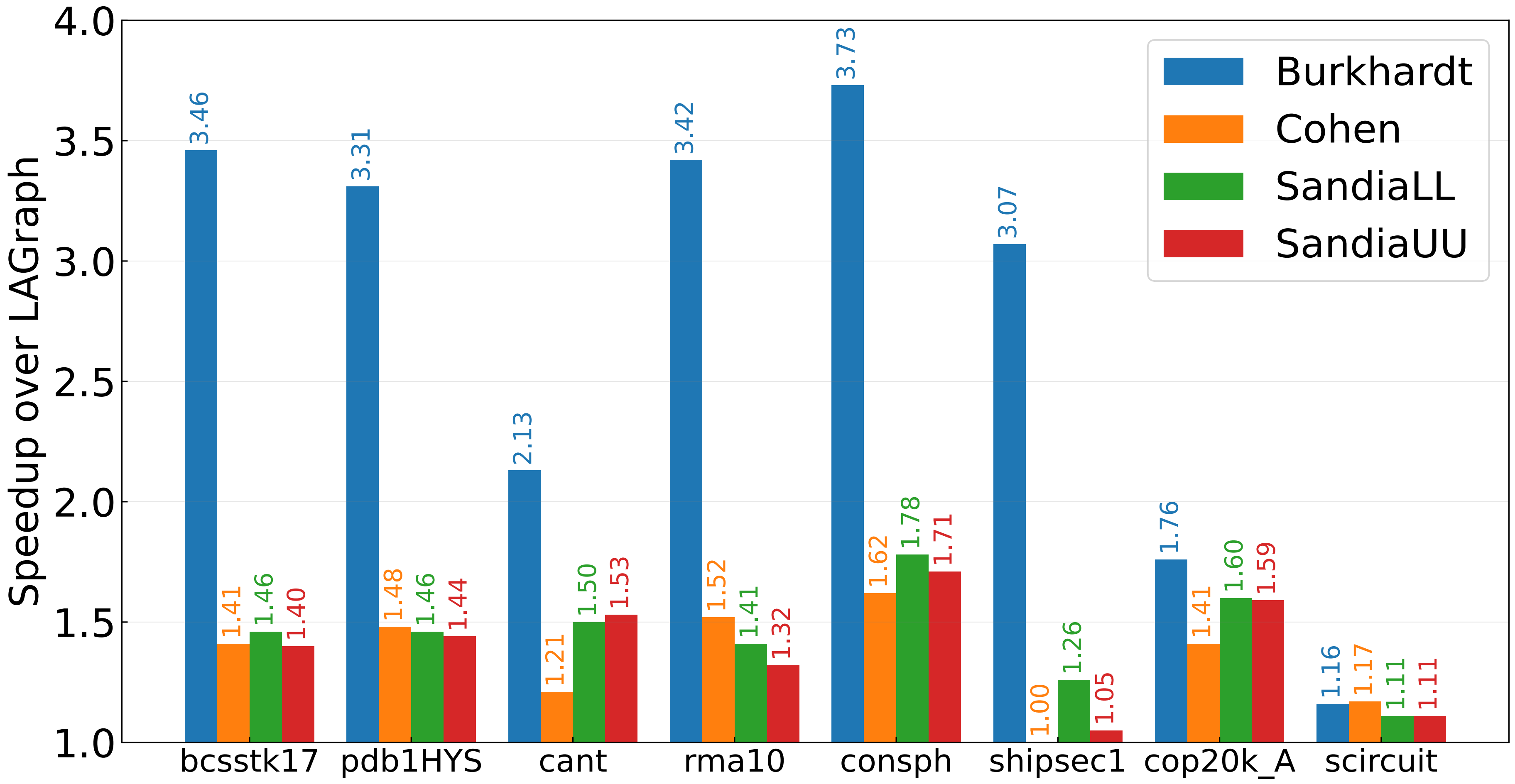
- Number of Triangles in a graph, where a triangle is a set of three mutually adjacent vertices in a graph.
- Various linear algebra-based algorithms proposed for the triangle counting problem.
    - Burkhard algorithm: $ntri = sum\big((A\ @(+,\times)A).*\ A\big)/6$
    - Cohen algorithm: $ntri = sum\big((L\ @(+,\times)U).*\ A\big)/2$
    - SandiaLL algorithm: $ntri = sum\big((L\ @(+,\times)L).*\ L\big)$
    - SandiaUU algorithm: $ntri = sum\big((U\ @(+,\times)U).*\ U\big)$

Triangle Counting in COMET

```
def main() {
    #IndexLabel Declarations
    IndexLabel [a] = [?];
    IndexLabel [b] = [?];
    IndexLabel [c] = [?];

    #Tensor Declarations
    Tensor<double> A([a, b], {CSR});
    Tensor<double> L([a, c], {CSR});
    Tensor<double> U([c, b], {CSR});

    #Tensor Data Initialization
    A[a, b] = comet_read(0, 1); # standard matrix read
    L[a, c] = comet_read(0, 2); # lower triangular read
    U[c, b] = comet_read(0, 4); # upper triangular read

    #PlusTimes semiring
    var ntri = SUM((L[a, c] @(+,*) U[c, b]) .* A[a, b])/2;
}
```

$$ntri = sum\big((L\ @(+,\times)U).*\ A\big)/2$$

Results: Triangle Counting



Conclusions and future work

- A DSL for implementing graph algorithms using linear algebra operations.
  - Support for semirings and masking.
- Optimizations for efficient codegen of sparse operations.
  - Workspace transforms.
- Sparse linear algebra operations as building blocks for graph algorithms paves the way for compiler optimizations.
  - Target heterogeneous accelerators.

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Thank you

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(ARIAA)

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