# CSE 599 I Accelerated Computing -Programming GPUS

Parallel Pattern: Sparse Matrices

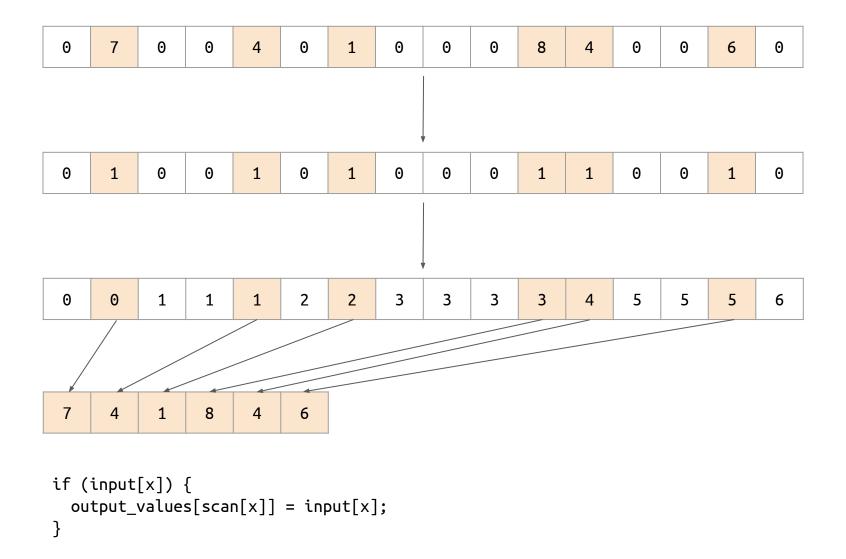
#### Objective

- Learn about various sparse matrix representations
- Consider how input data affects run-time performance of parallel sparse matrix algorithms
- Analyze trade-offs of different representations for various input types

# Sparse Vector Representation

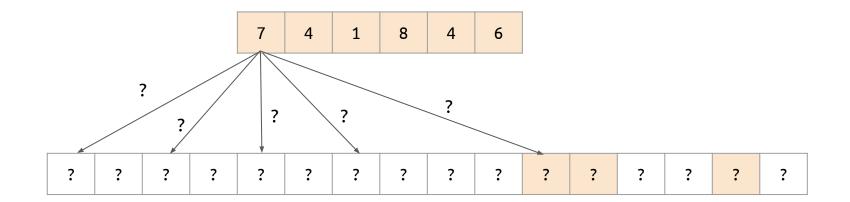
0	7	0	0	4	0	1	0	0	0	8	4	0	0	6	0	
_	-	_	_	_	_	_	_	_	_		-	_	_	_		

# Sparse Vector Representation



# Reconstructability

A successful sparse representation must allow for the reconstruction of the dense equivalent

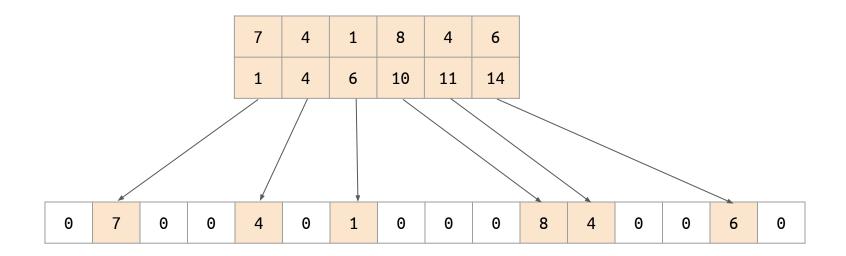


# Sparse Vector Representation

indices: values: if (input[x]) { output\_values[scan[x]] = input[x]; output indices[scan[x]] = x;

# Reconstructability

The reconstructability requirement imposes additional storage requirements on sparse representations



7

# Storage Requirements

N - number of elements in the vector

S - sparsity level [0 -1], 1 being fully-dense

Assume indices and values are the same size (e.g. 32-bit integers and floats)



#### Dense representation:

N words

7	4	1	8	4	6	
1	4	6	10	11	14	

#### Sparse representation:

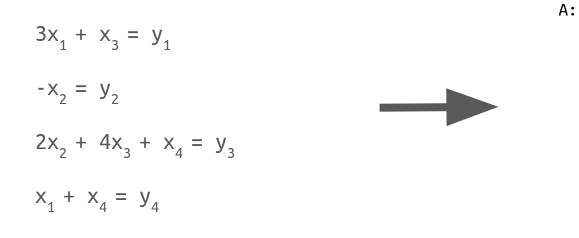
2NS words

The sparse representation only saves space if S < 1/2

#### Sparse Matrices

A matrix with a majority of nonzero elements

Frequently used to solve systems of linear equations with sparse dependencies



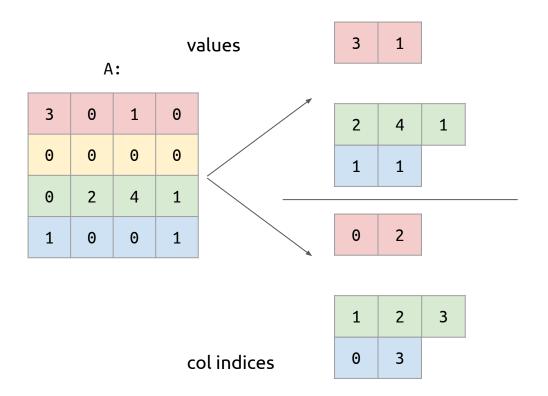
3	0	1	0
0	-1	0	0
0	2	4	1

$$Ax = y$$

#### Compressed Sparse Row (CSR) Format

High level idea: store each row as a sparse (row) vector

Each row is of variable length depending on the sparsity pattern

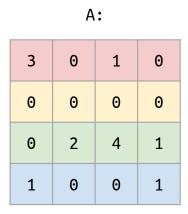


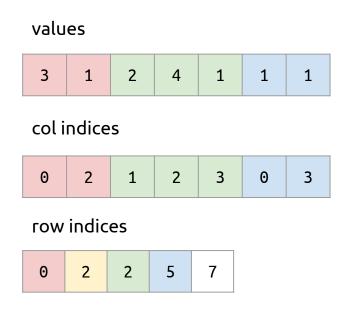
### Compressed Sparse Row (CSR) Format

High level idea: store each row as a sparse (row) vector

Each row is of variable length depending on the sparsity pattern

Additional storage is required to locate the start of each row





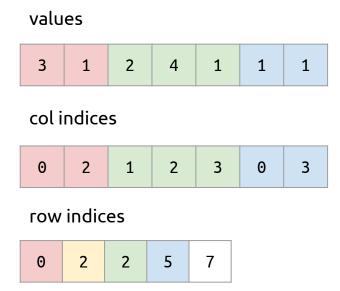
#### CSR Format Storage Requirement

M - number of rows in the matrix

N - number of columns in the matrix

S - sparsity level [0 -1], 1 being fully-dense

3	0	1	Θ
0	0	0	0
0	2	4	1
1	0	0	1



#### Dense representation

MN

#### Sparse representation

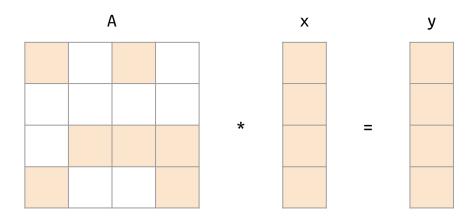
2MNS + M + 1

### Sparse Matrix-Vector Multiplication (SpMV)

We'll consider the application of multiplying a sparse matrix and a dense vector

Commonly used in graph-based applications

This is the core computation of iterative methods for solving sparse systems of linear equations:



#### A CSR Struct

```
struct SparseMatrixCSR {
    float * values;
    int * col_indices;
    int * row_indices;
    int M;
    int N;
};

We assume row_indices is of length M+1

We assume col_indices and values are of length row_indices[M]
```

You are allowed to pass structs (and classes) by value to a CUDA kernel!

# Sequential SpMV / CSR

```
void SpMV CSR(const SparseMatrixCSR A, const float * x, float * y) {
     for (int row = 0; row < A.M; ++row) {
          float dotProduct = 0;
          const int row_start = A.row_indices[row];
          const int row end = A.row indices[row+1];
          for (int element = row start; element < row_end; ++element) {</pre>
                dotProduct += A.values[element] * x[A.col indices[element]];
          }
                                                   This for loop iterates row end - row start times.
          y[row] = dotProduct;
                                                   row end - row start depends on the row
                                 Α
                                                      Χ
                                                                     У
```

# Parallel SpMV / CSR

As in dense matrix - vector multiplication, SpMV is data parallel

We can compute the dot product of each row of A with x in parallel

#### Parallel SpMV / CSR Kernel

```
__global__ void SpMV_CSR_kernel(const SparseMatrixCSR A, const float * x, float * y) {
     const int row = blockIdx.x * blockDim.x + threadIdx.x;
    if (row < A.M) {
          float dotProduct = 0;
          const int row start = A.row indices[row];
          const int row end = A.row indices[row+1];
          for (int element = row start; element < row end; ++element) {</pre>
               dotProduct += A.values[element] * x[A.col_indices[element]];
          y[row] = dotProduct;
```

### Parallel SpMV / CSR Kernel Shortcomings

#### 1. Non-coalesced memory access

```
dotProduct += A.values[element] * x[A.col_indices[element]];
```

Neighboring threads process neighboring rows, resulting in strided access

#### 2. Control flow divergence

Each row involves a variable amount of computation, which depends on the input

#### 3. Additional global memory reads

```
const int row_start = A.row_indices[row];
const int row_end = A.row_indices[row+1];
```

This will decrease our computation-to-global-memory-access (CGMA) ratio, which can have significant impact for smaller and / or highly - sparse matrices

Instead of "fixing" this kernel, let's consider other representations

#### **ELL Sparse Matrix Format**

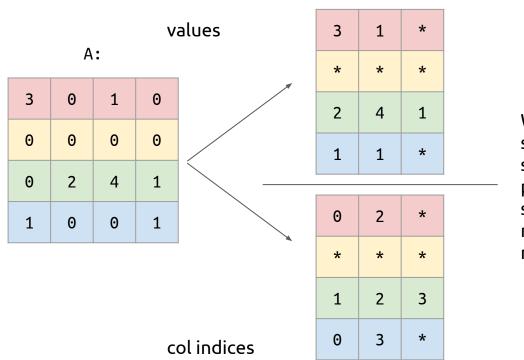
The name derives from the sparse matrix package in ELLPACK, a tool for solving elliptic boundary problems

ELL builds on CSR with two modifications:

- 1. Padding
- 2. Transposition

To form a padding representation, identify the longest row

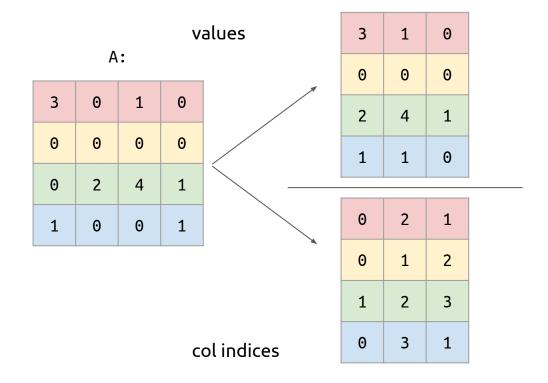
Allocate for each row enough space to hold the data for the longest row



We must pick a strategy for setting the padded values to satisfy the reconstructability requirement

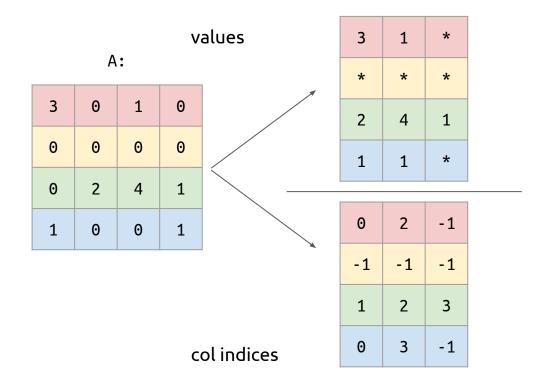
#### Option A:

Place zeros in values
Give the column index of an actual 0



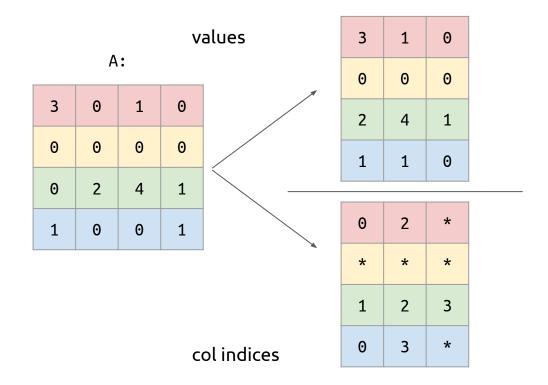
#### Option B:

Place an invalidating indicator into either array Requires algorithmic adjustment



#### Option B:

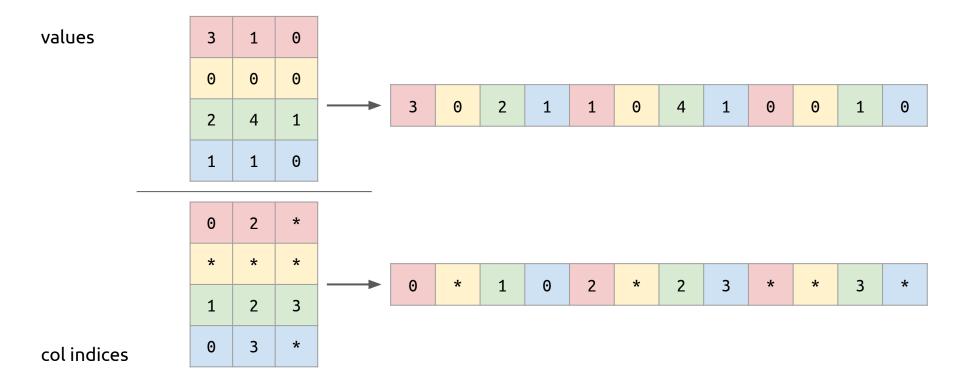
Place an invalidating indicator into either array Requires algorithmic adjustment



#### **Transposition**

Store the sparsified matrix in a column-major format (i.e. all elements in the same column are in contiguous memory locations)

This is the default for FORTRAN, but not for C



#### Storage Requirements

- M number of rows in the matrix
- N number of columns in the matrix
- **K** number of nonzero entries in the densest row
- S sparsity level [0 -1], 1 being fully-dense

Format	Storage Requirement (words)
Dense	MN
Compressed Sparse Row (CSR)	2MNS + M + 1
ELL	2MK

ELL only saves space if K < N / 2

#### An ELL Struct

```
struct SparseMatrixELL {
    float * values;
    int * col_indices;
    int M;
    int N;
    int K;
};
We assume col_indices and values are of length M * K;
```

### Parallel SpMV / ELL Kernel (Option A)

```
global void SpMV ELL kernel(const SparseMatrixELL A, const float * x, float * y) {
   const int row = blockIdx.x * blockDim.x + threadIdx.x;
   if (row < A.M) {
         float dotProduct = 0;
        for (int element = 0; element < A.K; ++element) {</pre>
              const int elementIndex = row + element* A.M;
              dotProduct += A.values[elementIndex] * x[A.col_indices[elementIndex]];
        y[row] = dotProduct;
                                              Global memory access depends on row, which has
                                              consecutive values for consecutive threadIdx.x
```

All threads iterate the same number of times

}

Global memory access for row indices is no longer required

#### Parallel SpMV / ELL Kernel (Option B)

```
__global__ void SpMV_ELL_kernel(const SparseMatrixELL A, const float * x, float * y) {
     const int row = blockIdx.x * blockDim.x + threadIdx.x;
     if (row < A.M) {
          float dotProduct = 0;
          for (int element = 0; element < A.K; ++element) {</pre>
               const int elementIndex = row + element* A.M;
               if (!A.values[elementIndex]) {
                     dotProduct += A.values[elementIndex] * x[A.col_indices[elementIndex]];
                                                We've re-introduced control flow divergence
                                                On the other hand, we avoid multiplication by 0
          y[row] = dotProduct;
```

# SpMV / ELL Kernel Shortcomings

This kernel will perform very well for matrices with similarly-dense rows

This approach is not equally well suited to all possible inputs

Consider a  $1000 \times 1000$  matrix with sparsity level 0.01:

- There are 1000 \* 1000 \* 0.01 = 10,000 multiply / adds to do
- If the densest row has 200 nonzero values, then the kernel will perform 1000 \* 200 = 200,000 multiply adds
- By using an ELL representation, we have increased the amount of computation AND memory access by 20x
- This is really bad worst-case performance!

### The Coordinate (COO) Format

High-level idea: store both the column index AND row index for every nonzero

This introduces additional storage for the extra index

There is no longer any required ordering for the elements

3	0	1	0	values:	3	1	2	4	1	1	1
0	0	0	0	→ column indices:	0	2	1	2	2	0	2
0	2	4	1	Cotumn maices.	0	2	1	2	3	0	3
1	0	0	1	row indices:	0	0	2	2	2	3	3

### The Coordinate (COO) Format

High-level idea: store both the column index AND row index for every nonzero

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3	0	1	0	values:	1	2	1	3	4	1	1
0	0	0	0	→ column indices:		1	2	0	2	2	2
0	2	4	1	Cotaliii ilidices.	0	1	3	0		3	
1	0	0	1	row indices:	3	2	2	0	2	3	0

#### Storage Requirements

- M number of rows in the matrix
- N number of columns in the matrix
- **K** number of nonzero entries in the densest row
- S sparsity level [0 -1], 1 being fully-dense

Format	Storage Requirement (words)					
Dense	MN					
Compressed Sparse Row (CSR)	2MNS + M + 1					
ELL	2MK					
Coordinate (COO)	3MNS					

COO only saves space if S < 1 / 3

#### A COO Struct

```
struct SparseMatrixC00 {
    float * values;
    int * col_indices;
    int * row_indices;
    int M;
    int N;
    int count;
};
```

We assume row\_indices, col\_indices, and values are of length count

# Sequential SpMV / COO

```
void SpMV_COO(const SparseMatrixCOO A, const float * x, float * y) {
    for (int element = 0; element < A.count; ++element) {
        const int column = A.col_indices[element];
        const int row = A.row_indices[element];
        y[row] += A.values[element] * x[column];
    }
}</pre>
```

This is a very satisfyingly simple function

Compared to the sequential SpMV / CSR, the sequential SpMN / COO doesn't waste time with fully-zero rows

# Parallel SpMV / COO

```
__global__ void SpMV_COO_kernel(const SparseMatrixCOO A, const float * x, float * y) {
    for (int element = threadIdx.x + blockIdx.x * blockDim.x;
        element < A.count;
        element += blockDim.x * gridDim.x) {
        const int column = A.col_indices[element];
        const int row = A.row_indices[element];

        y[row] += A.values[element] * x[column];
    }
    Output interference!</pre>
```

# Parallel SpMV / COO

```
__global__ void SpMV_COO_kernel(const SparseMatrixCOO A, const float * x, float * y) {
    for (int element = threadIdx.x + blockIdx.x * blockDim.x;
        element < A.count;
        element += blockDim.x * gridDim.x) {
        const int column = A.col_indices[element];
        const int row = A.row_indices[element];
        atomicAdd(&y[row], A.values[element] * x[column]);
    }
}</pre>
```

Switching to an atomic addition will make the output of this kernel correct...

It will also serialize a potentially large number of writes

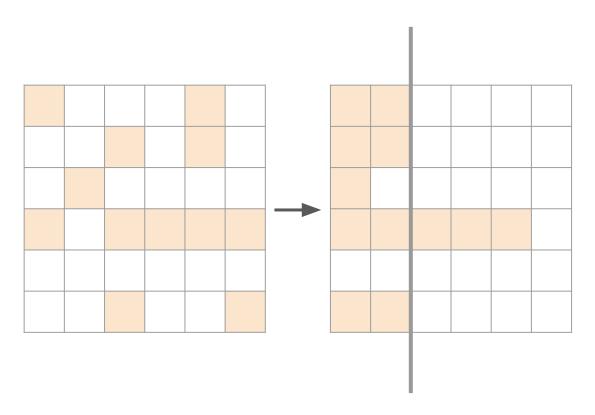
We could solve this using techniques from the histogram pattern (i.e. privitization)

We'll note that this representation is better suited to sequential hardware and take a different approach

# Hybrid ELL / COO Representation

High-level idea: place nonzeros from the densest rows in a COO sparse matrix, leading to a more efficient ELL representation for the remainder

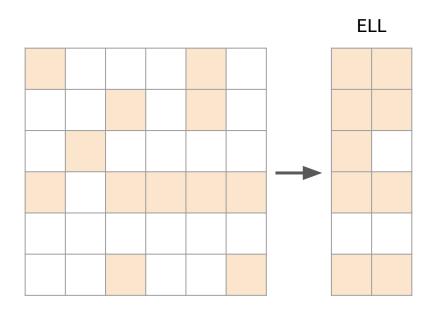
Each element will be stored in the ELL or the COO matrix, not both



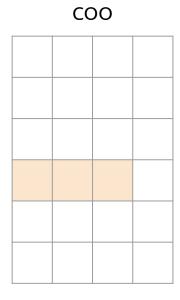
# Hybrid ELL / COO Representation

High-level idea: place nonzeros from the densest rows in a COO sparse matrix, leading to a more efficient ELL representation for the remainder

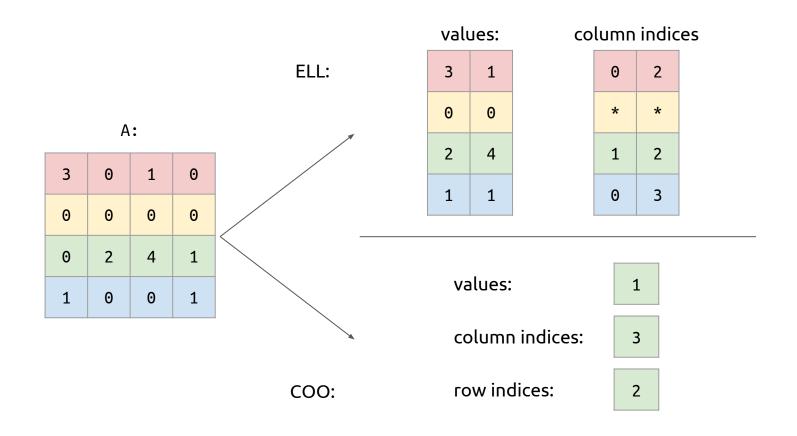
Each element will be stored in the ELL or the COO matrix, not both



2 \* 6 \* 2 = 24 words



# Hybrid ELL / COO Representation



### Storage Requirements

- M number of rows in the matrix
- N number of columns in the matrix
- **K** number of nonzero entries in the densest row
- S sparsity level [0 -1], 1 being fully-dense

Format	Storage Requirement (words)
Dense	MN
Compressed Sparse Row (CSR)	2MNS + M + 1
ELL	2MK
Coordinate (COO)	3MNS
Hybrid ELL / COO (HYB)	It's complicated!

### Storage Requirements

- M number of rows in the matrix
- N number of columns in the matrix
- **K** number of nonzero entries in the densest row
- S sparsity level [0 -1], 1 being fully-dense

Format	Storage Requirement (words)
Dense	MN
Compressed Sparse Row (CSR)	2MNS + M + 1
ELL	2MK
Coordinate (COO)	3MNS
Hybrid ELL / COO (HYB)	> 3MNS, < 2MK

# Hybrid ELL / COO SpMV

- Perform the SpMV / ELL in parallel on the GPU
  - As we've seen, the ELL format is handled efficiently by the GPU as long as the rows are roughly the same density
- Perform the SpMV / COO sequentially on the CPU
  - The irregular memory access and output interference of the SpMV /
     COO is better suited to the CPU with it's large cache memory

Be careful that the time spent building a more complicated representation is justified by the usage

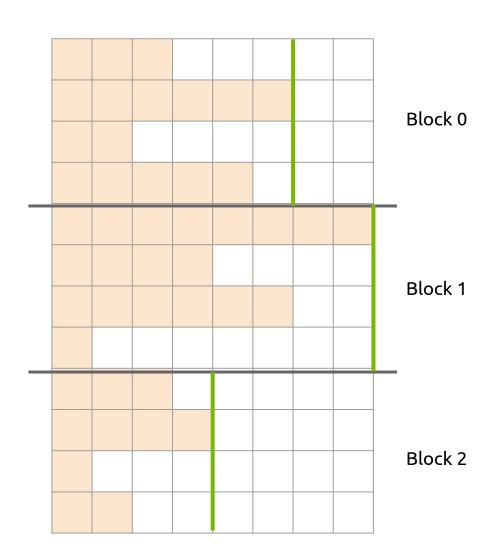
# SpMV / HYB Host Code

```
void hybridSpMV(const float * A, const int M, const int N const float * x, float * y) {
     float * d_y;
     float * d x;
     float * y ELL;
     SparseMatrixELL d_A_ELL;
     SparseMatrixCOO A_COO;
     // build sparse matrix representations, allocate / initialize host and device memory
     // launch ELL kernel
     SpMV_ELL_kernel<<<(A.M + 127)/128,128>>>(d_A_ELL, d_x, d_y);
     // copy device result back to host
     cudaMemcpy(y_ELL, d_y, A.N * sizeof(float), cudaMemcpyDeviceToHost );
     // perform host computation
                                                                           This function waits for the
     SpMV_COO(A_COO, x, y_ELL);
                                                                           kernel launch to complete
```

# SpMV / HYB Host Code

```
void hybridSpMV(const float * A, const int M, const int N const float * x, float * y) {
     float * d_y;
     float * d x;
     float * y ELL;
     SparseMatrixELL d_A_ELL;
     SparseMatrixCOO A_COO;
     // build sparse matrix representations, allocate / initialize host and device memory
     // launch ELL kernel
     SpMV ELL kernel <<< (A.M + 127)/128,128 >>> (d A ELL, d x, d y);
     // perform host computation
     SpMV_COO(A_COO, x, y);
                                                          This computation might happen "for free"!
     // copy device result back to host
     cudaMemcpy(y_ELL, d_y, A.N * sizeof(float) );
     for (int i = 0; i < A.N; ++i) {
          y[i] += y_ELL[i];
```

### **CSR** revisited



In the parallel SpMV / CSR kernel running on a CUDA device, the output is computed in blocks

The runtime of each block is determined by the densest row in the block

# Jagged Diagonal Storage (JDS) Format

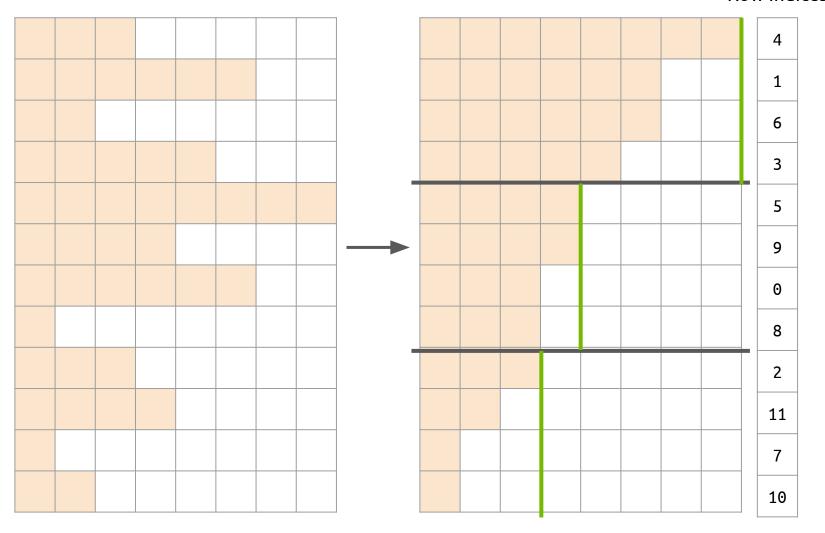
High-level idea: Group similarly dense rows into evenly-sized partitions, and represent each section independently using either CSR or ELL

This can be done by sorting rows by density

We need to store the original indices of the sorted rows to satisfy the reconstructability requirement

# Jagged Diagonal Storage (JDS) Format

#### **Row Indices**

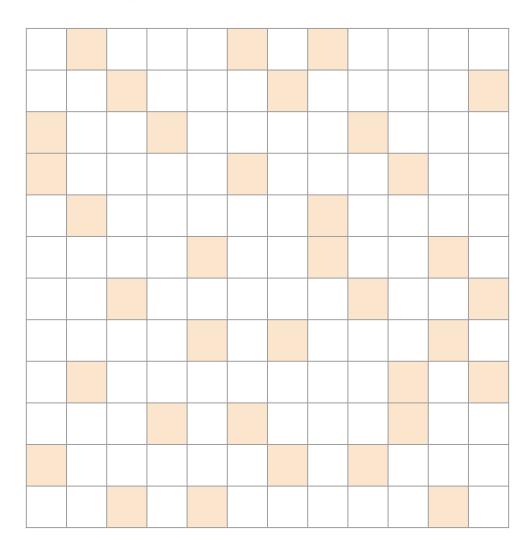


# Jagged Diagonal Storage (JDS) Format

The JDS groups can be naturally mapped to CUDA blocks

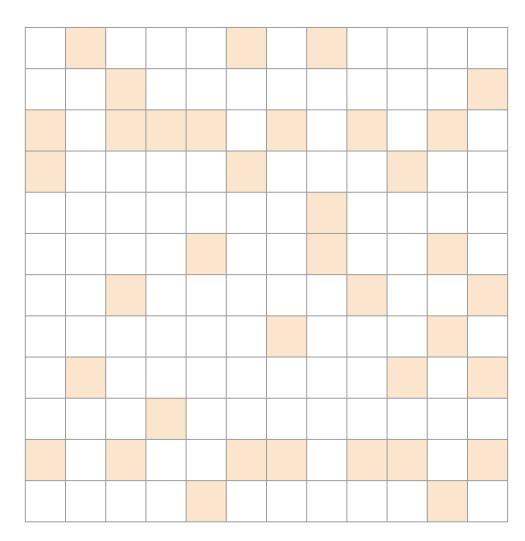
While the blocks may require variable amounts of computation, threads within the same block will do similar amounts of computation

This will help maximize bandwidth

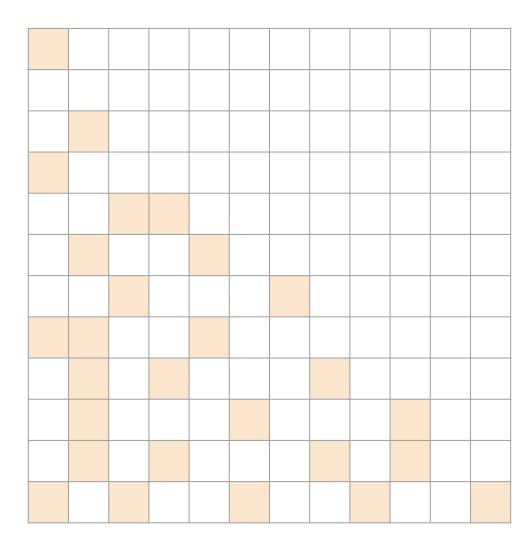


Roughly random?

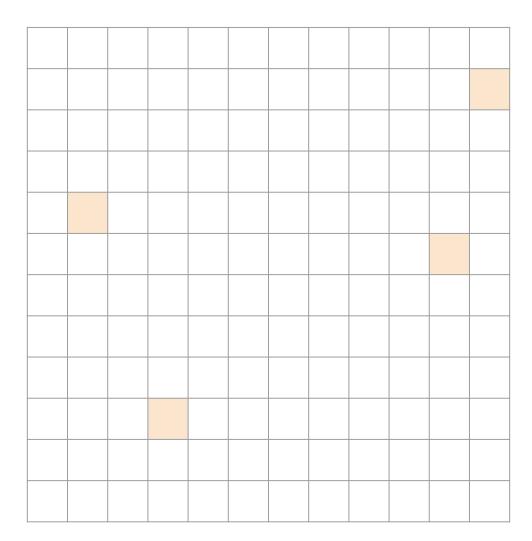
Roughly random, but with more variance in the sparsity between rows?



Probably best with a hybrid COO / ELL representation



Roughly triangular?



Extremely sparse?

## Other Sparse Matrix Representations

#### Diagonal (DIA):

- Stores only a sparse set of dense diagonal vectors
- For each diagonal, the offset from the main diagonal is stored

#### Packet (PKT):

- Reorders rows and columns to concentrate nonzeros into roughly diagonal submatrices
- This improves cache performance as nearby rows access nearby x elements

#### Dictionary of Keys (DOK):

- Matrix is stored as a map from (row,column) index pairs to values
- This can be useful for building or querying a sparse matrix, but iteration is slow

#### Compressed Sparse Column (CSC):

- Like CSR, but stores a dense set of sparse column vectors
- Useful for when column sparsity is much more regular than row sparsity

#### Blocked CSR

- The matrix is divided into blocks stored using CSR with the indices of the upper left corner
- Useful for block-sparse matrices

### • Additional Hybrid Methods:

- For example, DIA is very inefficient when there are a small number of mostly-dense diagonals, but a few additional sparse entries
- o In this case, a hybrid DIA / COO or DIA / CSR representation can be used

## Conclusion / Takeaways

- Sparse matrices are hard!
- There are a lot of ways to represent sparse matrices
- Different representations have different storage requirements
- The storage requirements depend differently on the sparsity pattern
- There is sometimes a need to safeguard against worst-case input
- There is often a trade-off between regularity and efficiency
- Some representations are better suited to certain hardware than others
- It can be difficult to achieve a high compute-to-global-memory-access ratio
   (CGMA) when it comes to sparse matrices
  - The above is especially true in the case of SpMV, where each row participates in a separate computation

# Appendix: Sparse Matrix Libraries

If I'm never going to implement my own sparse matrix multiplication, who cares?

 Dealing with data-dependent performance and avoiding irregularity are common issues in massively-parallel programming

• If it's hard for you to write sparse matrix algorithms that work efficiently in all cases, it's hard for library implementers as well!

 Knowing the trade-offs can help you make better use of sparse matrix libraries

https://developer.nvidia.com/cusparse

cuSPARSE is an nVidia library implemented a set of basic linear algebra subroutines (BLAS)

#### **Key Features**

- Supports dense, COO, CSR, CSC, ELL/HYB and Blocked CSR sparse matrix formats
- Level 1 routines for sparse vector x dense vector operations
- Level 2 routines for sparse matrix x dense vector operations
- Level 3 routines for sparse matrix x multiple dense vectors (tall matrix)
- Routines for sparse matrix by sparse matrix addition and multiplication
- Conversion routines that allow conversion between different matrix formats
- Sparse Triangular Solve
- Tri-diagonal solver
- Incomplete factorization preconditioners ilu0 and ic0

cuSPARSE offers a fairly low-level API

For the most part, operations are performed on raw data buffers:

Full documentation at: <a href="http://docs.nvidia.com/cuda/cusparse">http://docs.nvidia.com/cuda/cusparse</a>

```
// create the cuSPARSE handle
cusparseCreate(&handle);
// Allocate device memory for vectors and the dense form of matrix A
// Construct a descriptor of the matrix A
cusparseCreateMatDescr(&descr);
cusparseSetMatType(descr, CUSPARSE_MATRIX_TYPE_GENERAL);
cusparseSetMatIndexBase(descr, CUSPARSE_INDEX_BASE_ZERO);
// Transfer the input vectors and dense matrix A to the device
// Compute the number of non-zero elements in A
cusparseSnnz(handle, CUSPARSE_DIRECTION_ROW, M, N, descr, dA, M, dNnzPerRow, &totalNnz);
// Allocate device memory to store the sparse CSR representation of A
// Convert A from a dense format to a CSR format, using the GPU
cusparseSdense2csr(handle, M, N, descr, dA, M, dNnzPerRow, dCsrValA, dCsrRowPtrA, dCsrColIndA);
// Perform matrix-vector multiplication with the CSR-format matrix A
cusparseScsrmv(handle, CUSPARSE_OPERATION_NON_TRANSPOSE, M, N, totalNnz, &alpha, descr, dCsrValA,
               dCsrRowPtrA, dCsrColIndA, dX, &beta, dY);
// Copy the result back of the host
cudaMemcpy(Y, dY, sizeof(float) * M, cudaMemcpyDeviceToHost);
```

### https://cusplibrary.github.io/

#### What is CUSP?

Cusp is a library for sparse linear algebra and graph computations based on Thrust. Cusp provides a flexible, high-level interface for manipulating sparse matrices and solving sparse linear systems.

#### CUSP is an open source project

It is focused on solving linear systems, providing a number of conjugate-gradient solvers

### Supported matrix types:

- COO
- CSR
- DIA
- ELL
- HYB

```
#include <cusp/csr_matrix.h>
#include <cusp/hyb_matrix.h>
int main() {

    // Allocate storage for a 5 by 8 sparse matrix in CSR format with 12
    // nonzero entries on the host
    cusp::csr_matrix<int,float,cusp::host_memory> csr_host(5,8,12);

    // Transfer the matrix to the device
    cusp::csr_matrix<int,float,cusp::device_memory> csr_device(csr_host);

    // Convert the matrix to HYB format on the device
    cusp::hyb_matrix<int,float,cusp::device_memory> csr_device(csr_device);
}
```

```
#include <cusp/csr_matrix.h>
#include <cusp/hyb_matrix.h>
int main() {

    // Allocate storage for a 5 by 8 sparse matrix in CSR format with 12
    // nonzero entries on the host
    cusp::csr_matrix<int,float,cusp::host_memory> csr_host(5,8,12);

    // Transfer the matrix to the device
    cusp::csr_matrix<int,float,cusp::device_memory> csr_device(csr_host);

    // Convert the matrix to HYB format on the device
    cusp::hyb_matrix<int,float,cusp::device_memory> csr_device(csr_device);
}
```

```
// include the csr matrix header file
#include <cusp/csr matrix.h>
#include <cusp/print.h>
int main() {
     // allocate storage for (4,3) matrix with 4 nonzeros
     cusp::csr_matrix<int,float,cusp::host_memory> A(4,3,6);
     // initialize matrix entries on host
     A.row offsets[0] = 0; // first offset is always zero
     A.row offsets[1] = 2;
     A.row offsets[2] = 2;
     A.row offsets[3] = 3;
     A.row_offsets[4] = 6; // last offset is always num entries
     A.column indices[0] = 0; A.values[0] = 10;
     A.column indices[1] = 2; A.values[1] = 20;
     A.column indices[2] = 2; A.values[2] = 30;
     A.column indices[3] = 0; A.values[3] = 40;
     A.column indices[4] = 1; A.values[4] = 50;
     A.column indices[5] = 2; A.values[5] = 60;
     // A now represents the following matrix
     // [10 0 20]
     [0 0 0]
     // [0 0 30]
      // [40 50 60]
      // copy to the device
     cusp::csr_matrix<int,float,cusp::device_memory> B(A);
     cusp::print(B);
}
```

### Provides a number of matrix operations:

- Matrix addition
- Transposition
- SpMV
- Matrix-matrix multiplication
- Generic element-wise operations
- etc.

### Sources

Bell, Nathan, and Michael Garland. Efficient sparse matrix-vector multiplication on CUDA. Vol. 2. No. 5. Nvidia Technical Report NVR-2008-004, Nvidia Corporation, 2008.

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Hwu, Wen-mei, and David Kirk. "Programming massively parallel processors." Special Edition 92 (2009).