Computational Science on Many-Core Architectures

360.252

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Agenda for Today

Exercise 4 Recap

Finite Differences

Recap: Prefix Sums

Sequential to Parallel: ILU Example

Exercise 5

Exercise 4 Recap

Feedback Time

- How was your experience?

Exercise 4 Recap

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- You should have received links to points for course last week

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Vector Iterations

```
__kernel__ void option1(double *x, int N, ...) {
for (int row = blockDim.x * blockIdx.x + threadIdx.x;
      row < N;
      row += gridDim.x * blockDim.x) { ... }
}
option1<<<256, 256>>>(x, N, ...);  // arbitrary grid/block dim
```

```
__kernel__ void option2(double *x, int N, ...) {
  if (blockDim.x*blockIdx.x + threadIdx.x < N) { ... }
}
option2<<<N/blocksize + 1, blocksize>>>(x, N, ...); // beware!
```

Finite Differences

Discrete Poisson Equation

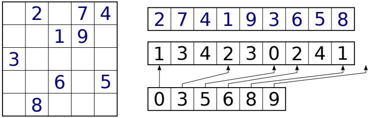
- Rectangular grid
- Assume homogeneous grid spacing h
- Discretize each coordinate direction separately

$$
\begin{aligned}
\Delta u(x,y) &= u_{xx}(x,y) + u_{yy}(x,y) \\
&\approx \frac{u(x-h,y) - 2u(x,y) + u(x+h,y)}{h^2} + \frac{u(x,y-h) - 2u(x,y) + u(x,y+h)}{h^2} \\
&= \frac{u(x-h,y) + u(x+h,y) - 4u(x,y) + u(x,y-h) + u(x,y+h)}{h^2} \\
&=: \Delta_h u(x,y)
\end{aligned}
$$

Finite Differences

System Matrix Structure

- Interior nodes have 5 nonzero entries
- Boundary nodes have 1 to 4 nonzero entries
- Problem: CSR format requires offset index for each row



Matrix CSR

Finite Differences

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- Boundary nodes have 1 to 4 nonzero entries
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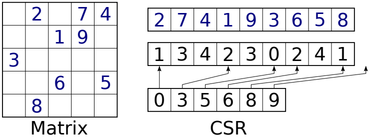


Generic GPU matrix assembly skeleton

1. Count the nonzero entries for each row
2. Deduce offsets for CSR
3. Populate column and values arrays

Finite Differences

Step 1: Count Nonzeros for an $N \times M$ grid

```
__kernel__ void count_nnz(int *row_offsets, int N, ...) {
for (int row = blockDim.x * blockIdx.x + threadIdx.x;
      row < N*M;
      row += gridDim.x * blockDim.x)
    {
        int nnz_for_this_node = 1;
        int i = row / N;
        int j = row % N;

        if (i > 0) nnz_for_this_node += 1;
        if (j > 0) nnz_for_this_node += 1;
        if (i < N-1) nnz_for_this_node += 1;
        if (j < M-1) nnz_for_this_node += 1;

        row_offsets[row] = nnz_for_this_node;
      }
}
```

Parallel Primitives

Prefix Sum

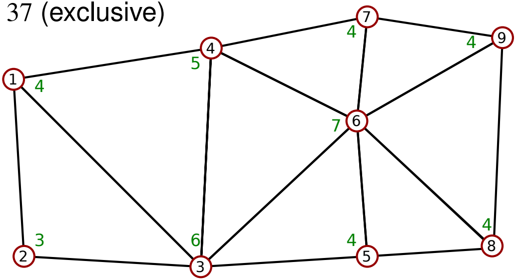
- Inclusive: Determine $y_i = \sum_{k=1}^{i} x_k$
- Exclusive: Determine $y_i = \sum_{k=1}^{i-1} x_k$, $y_1 = 0$

Example

- x: 4, 3, 6, 5, 4, 7, 4, 4, 4
- y: 4, 7, 13, 18, 22, 29, 33, 37, 41 (inclusive)
- y: 0, 4, 7, 13, 18, 22, 29, 33, 37 (exclusive)

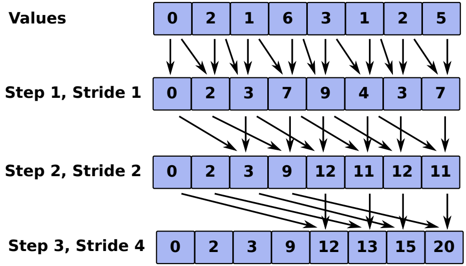
Applications

- Sparse matrix setup
- Graph algorithms



Parallel Primitives

Prefix Sum Implementation




```
for(int stride = 1; stride < blockDim.x; stride *= 2)
{
  __syncthreads();
  shared_m[threadIdx.x] = my_value;
  __syncthreads();
  if (threadIdx.x >= stride)
    my_value += shared_m[threadIdx.x - stride];
}
__syncthreads();
shared_m[threadIdx.x] = my_value;
```

Finite Differences

Step 3: Assembly for an $N \times M$ grid

```
__kernel__ void assembleA(int *row_offsets, int N, ...) {
for (int row = blockDim.x * blockIdx.x + threadIdx.x;
      row < N*M;
      row += gridDim.x * blockDim.x) {
        int i = row / N;
        int j = row % N;
        int this_row_offset = row_offsets[row];

        int index = i * N + j;
        col_indices[this_row_offset] = index;
        values[this_row_offset] = 4;
        this_row_offset += 1;

        if (i > 0) { /* similarly with correct index and value -1
            */ }
        if (j > 0) { /* similarly */ }
        if (i < N-1)  { /* similarly */ }
        if (j < M-1) { /* similarly */ }
      }
}
```

Other Discretizations

Finite Volumes

- Iterations over vertices: Similar to finite differences
- Beware of advanced schemes (depends)

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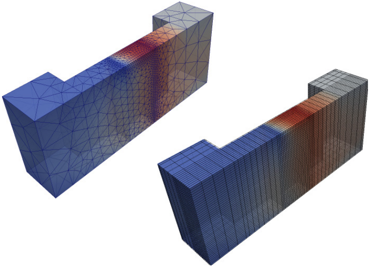
Finite Elements

- Iteration over elements (cells)
- BUT: write matrix entries associated with vertices
- $\Rightarrow$ Avoid race conditions
- More preparation required before we can address this



Next Step

Sequential to Parallel: ILU Example

(in preparation for Finite Element assembly strategies)

Parallel ILU

ILU - Basic Idea

- Factor sparse matrix $\boldsymbol{A} \approx \tilde{\boldsymbol{L}}\tilde{\boldsymbol{U}}$
- $\tilde{\boldsymbol{L}}$ and $\tilde{\boldsymbol{U}}$ sparse, triangular
- ILU0: Pattern of $\tilde{\boldsymbol{L}}$, $\tilde{\boldsymbol{U}}$ equal to $\boldsymbol{A}$
- ILUT: Keep k elements per row

Solver Cycle Phase

- Residual correction $\color{red}{\tilde{\boldsymbol{L}}}\color{black}\tilde{\boldsymbol{U}}x = z$
- Forward solve $\color{red}{\tilde{\boldsymbol{L}}}\color{black}y = z$
- Backward solve $\tilde{\boldsymbol{U}}x = y$
- Little parallelism in general

$$\begin{pmatrix}
5 & \times & \times & \times & & \times & \times & & \\
\color{red}\times & 3 & \times & & & & & & \\
\color{red}\times & \color{red}\times & 4 & \times & & & & & \\
\color{red}\times & & \color{red}\times & 5 & \times & \times & & & \times \\
 & & & \color{red}\times & 5 & \times & & \times & \times \\
\color{red}\times & & & \color{red}\times & \color{red}\times & 6 & \times & \times & \\
\color{red}\times & & & & & \color{red}\times & 3 & & \\
 & & & & \color{red}\times & \color{red}\times & & 4 & \times \\
 & & & \color{red}\times & \color{red}\times & & & \color{red}\times & 4
\end{pmatrix}$$

Parallel ILU

ILU Level Scheduling

- Build dependency graph
- Substitute as many entries as possible simultaneously
- Trade-off: Each step vs. multiple steps in a single kernel

$$
\begin{pmatrix}
5 & \times & \times & \times & & \times & \times & & \\
\times & 3 & \times & & & & & & \\
\times & \times & 4 & \times & & & & & \\
\times & & \times & 5 & \times & \times & & & \times \\
 & & & \times & 5 & \times & & \times & \times \\
\times & & & \times & \times & 6 & \times & \times & \\
\times & & & & & \times & 3 & & \\
 & & & & \times & \times & & 4 & \times \\
 & & & \times & \times & & & \times & 4
\end{pmatrix}
$$

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\times & \times & 4 & \times & & & & & \\
\times & & \times & 5 & \times & \times & & & \times \\
 & & & \times & 5 & \times & & \times & \times \\
\times & & & \times & \times & 6 & \times & \times & \\
\times & & & & & \times & 3 & & \\
 & & & & \times & \times & & 4 & \times \\
 & & & \times & \times & & & \times & 4
\end{pmatrix}
$$

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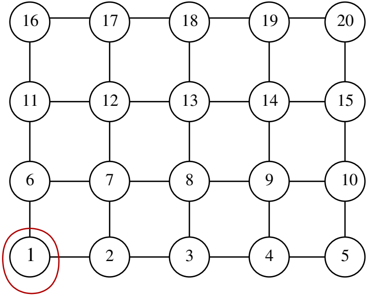
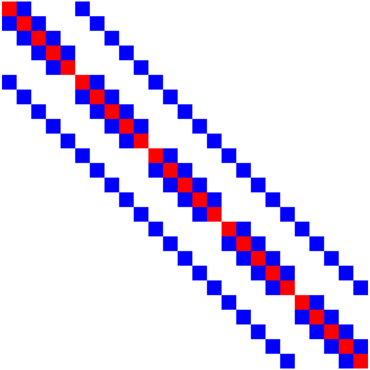
5 & \times & \times & \times & & \times & \times & & \\
\times & 3 & \times & & & & & & \\
\times & \times & 4 & \times & & & & & \\
\times & & \times & 5 & \times & \times & & & \times \\
 & & & \times & 5 & \times & & \times & \times \\
\times & & & \times & \times & 6 & \times & \times & \\
\times & & & & & \times & 3 & & \\
 & & & & \times & \times & & 4 & \times \\
 & & & \times & \times & & & \times & 4
\end{pmatrix}
$$

Parallel ILU

ILU Interpretation on Structured Grids

- 2d finite-difference discretization
- Substitution whenever all neighbors with smaller index computed
- Works particularly well in 3d





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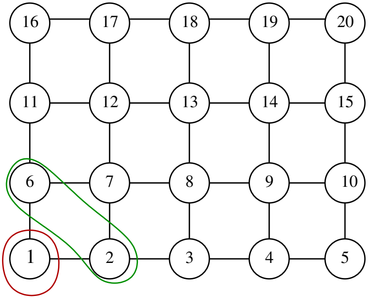

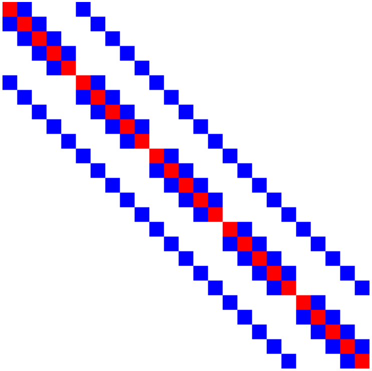

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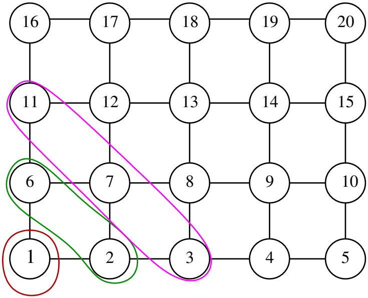

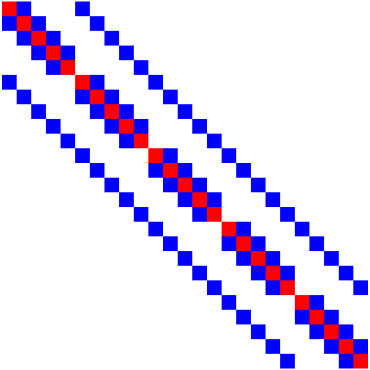

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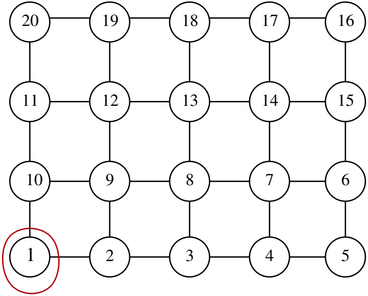

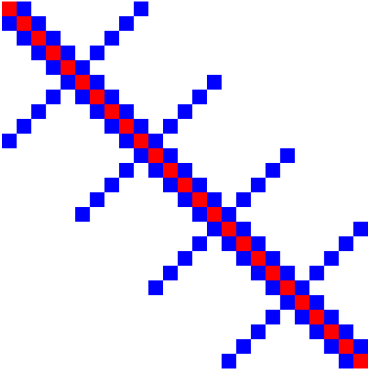

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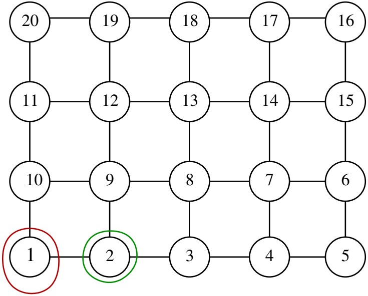

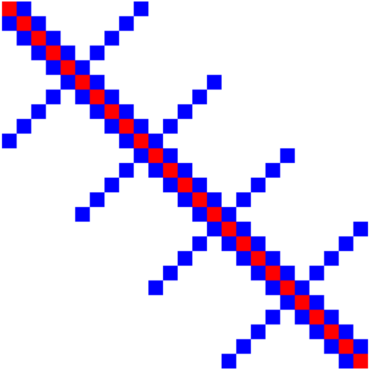

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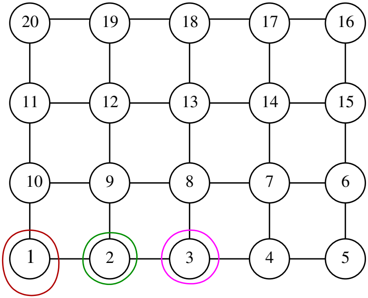

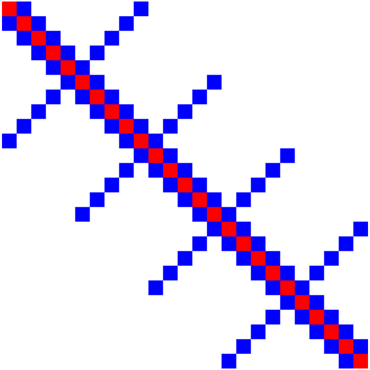

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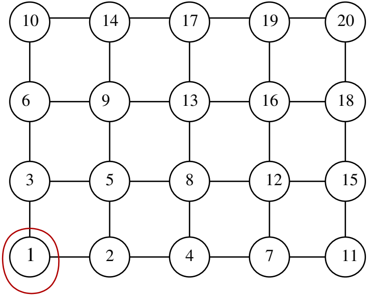

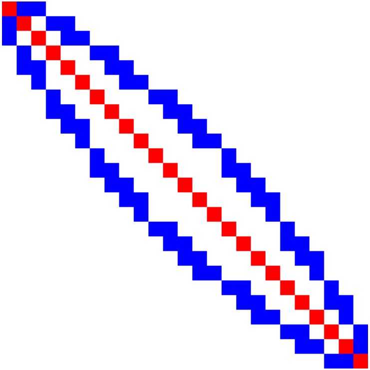

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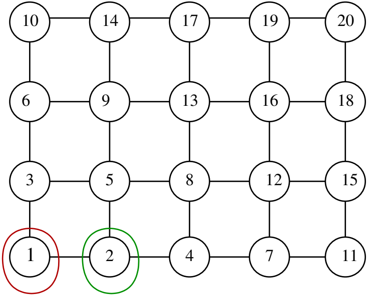

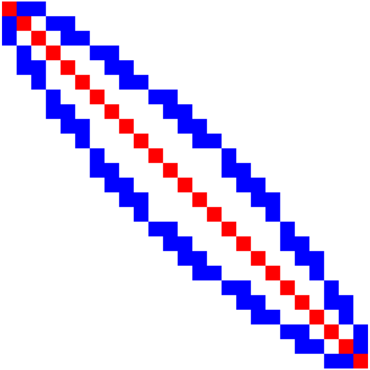

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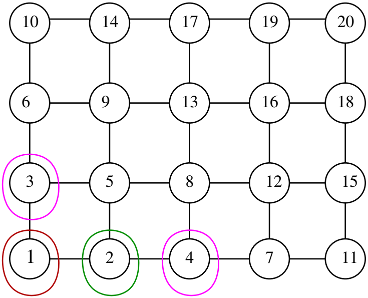

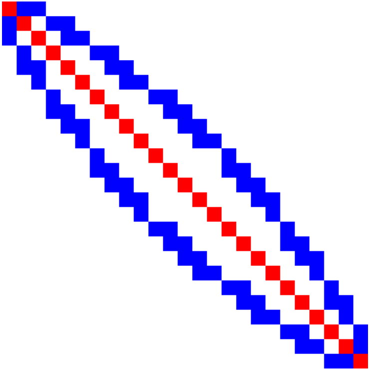

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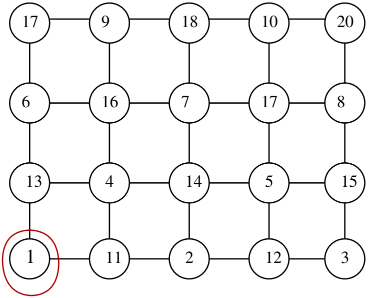

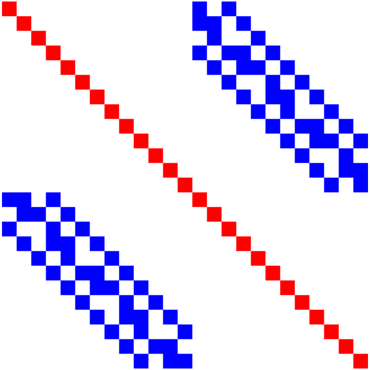

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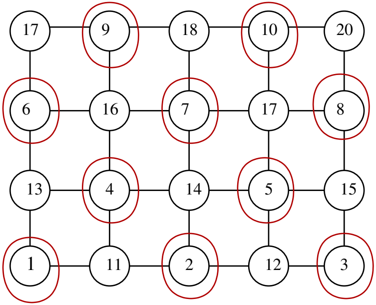

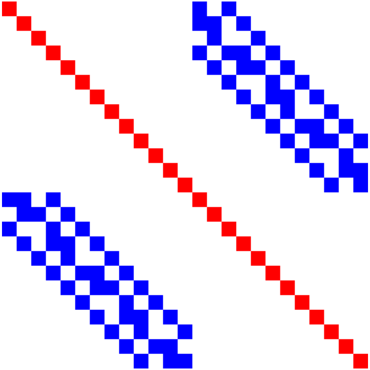

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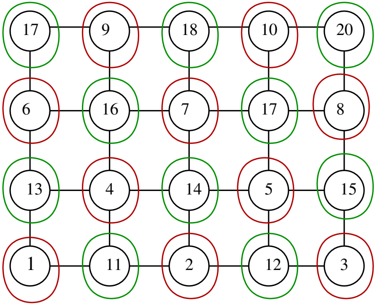

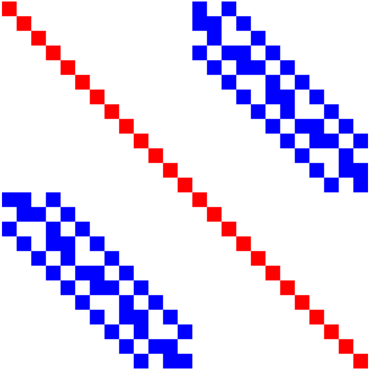

Parallel ILU - Innovation

Sequential

```
for i=2..n
  for k=1..i-1, (i,k)in A
```

$$a_{ik} = a_{ik}/a_{kk}$$

```
    for j=k+1..n, (i,j)in A
```

$$u_{ij} = a_{ij} - a_{ik}a_{kj}$$

Parallel

```
for (sweep = 1, 2, ...)
 parallel for (i,j)in A
   if (i > j)
```

$$l_{ij} = (a_{ij} - \sum_{k=1}^{j=1} l_{ik}u_{kj})/u_{jj}$$

```
   else
```

$$u_{ij} = a_{ij} - \sum_{k=1}^{=1} l_{ik}u_{kj}$$

Fine-Grained Parallel ILU Setup

- Proposed by Chow and Patel (SISC, vol. 37(2)) for CPUs and MICs
- Massively parallel (one thread per row)

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Fine-Grained Parallel ILU Setup

- Proposed by Chow and Patel (SISC, vol. 37(2)) for CPUs and MICs
- Massively parallel (one thread per row)

Preconditioner Application

- Truncated Neumann series:

$$\mathbf{L}^{-1} \approx \sum_{k=0}^{K} (\mathbf{I} - \mathbf{L})^k, \quad \mathbf{U}^{-1} \approx \sum_{k=0}^{K} (\mathbf{I} - \mathbf{U})^k$$

- Exact triangular solves not necessary

Exercises

Environment

- `https://gtx1080.360252.org/2020/ex5/`
- (Might receive visual updates and additional hints over the next days)
- Due: Tuesday, November 24, 2020 at 23:59pm

Hints and Suggestions

- Consider version control for locally developed code
- Please let me know of any bugs or issues