Computational Science on Many-Core Architectures

360.252

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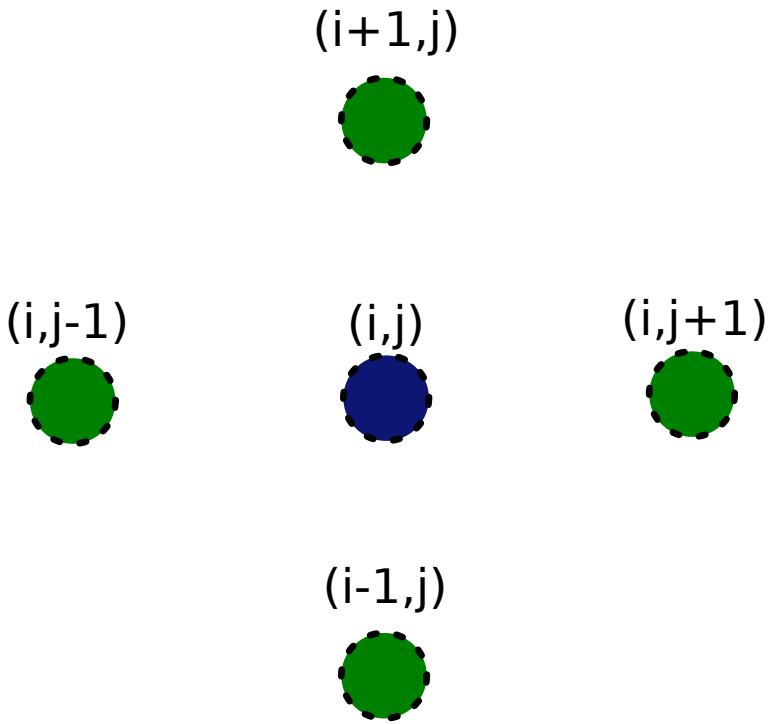
Finite Differences

Discrete Poisson Equation $-\Delta_h u(x,y) = f_h(x,y)$

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

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

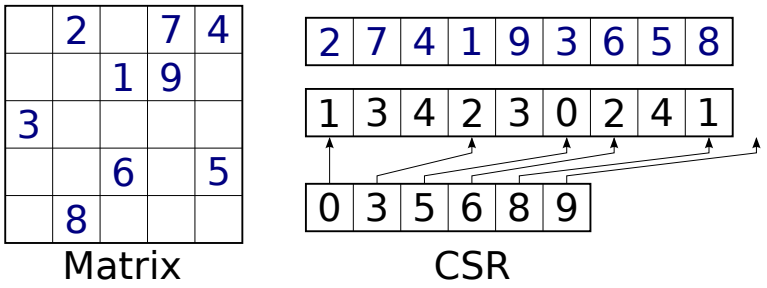
Finite Differences



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



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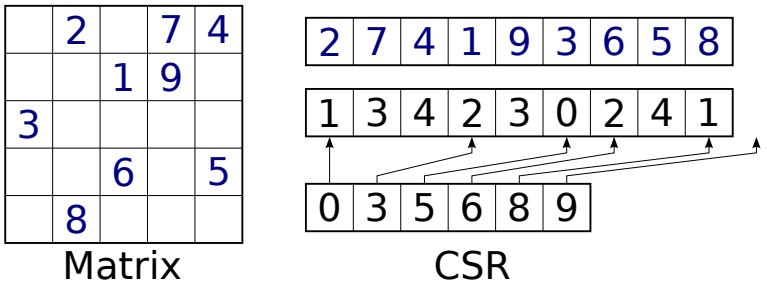


Generic GPU matrix assembly skeleton

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

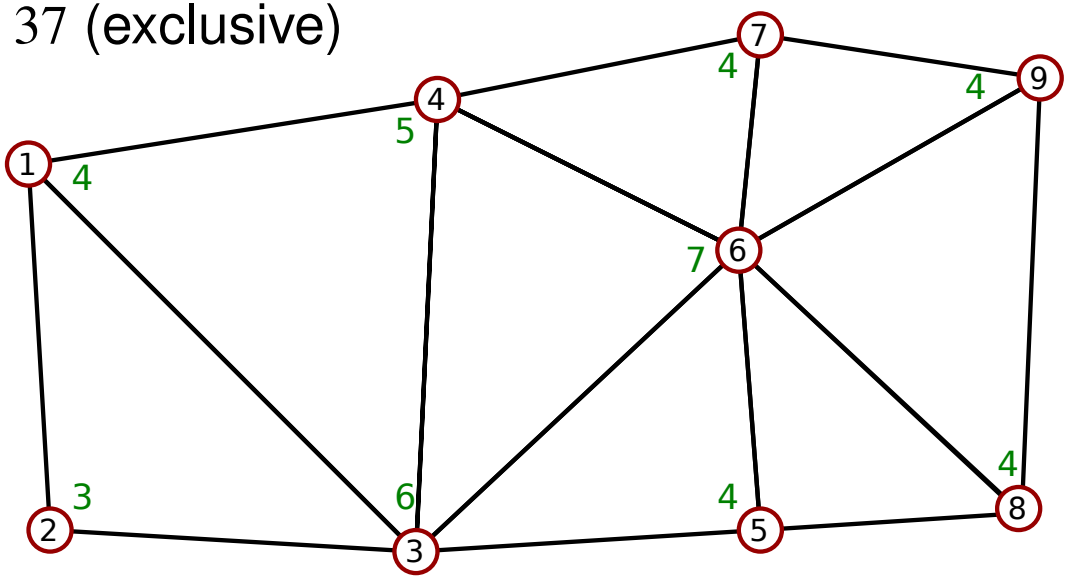
- Inclusive: Determine $y_i = \sum_{k=1}^{i} x_k$
- Exclusive: Determine $y_i = \sum_{k=1}^{i-1} x_k$, $y_1 = 0$

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)

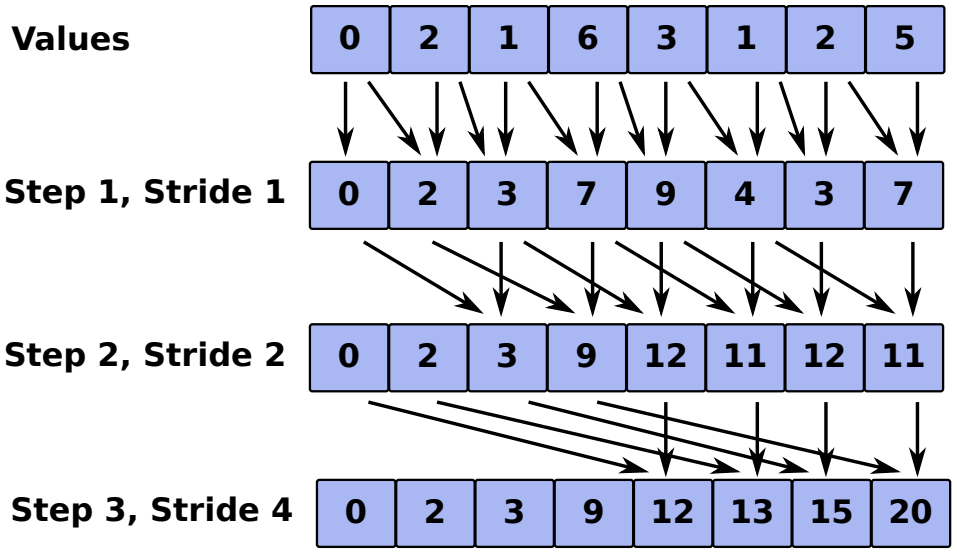
Applications

- 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

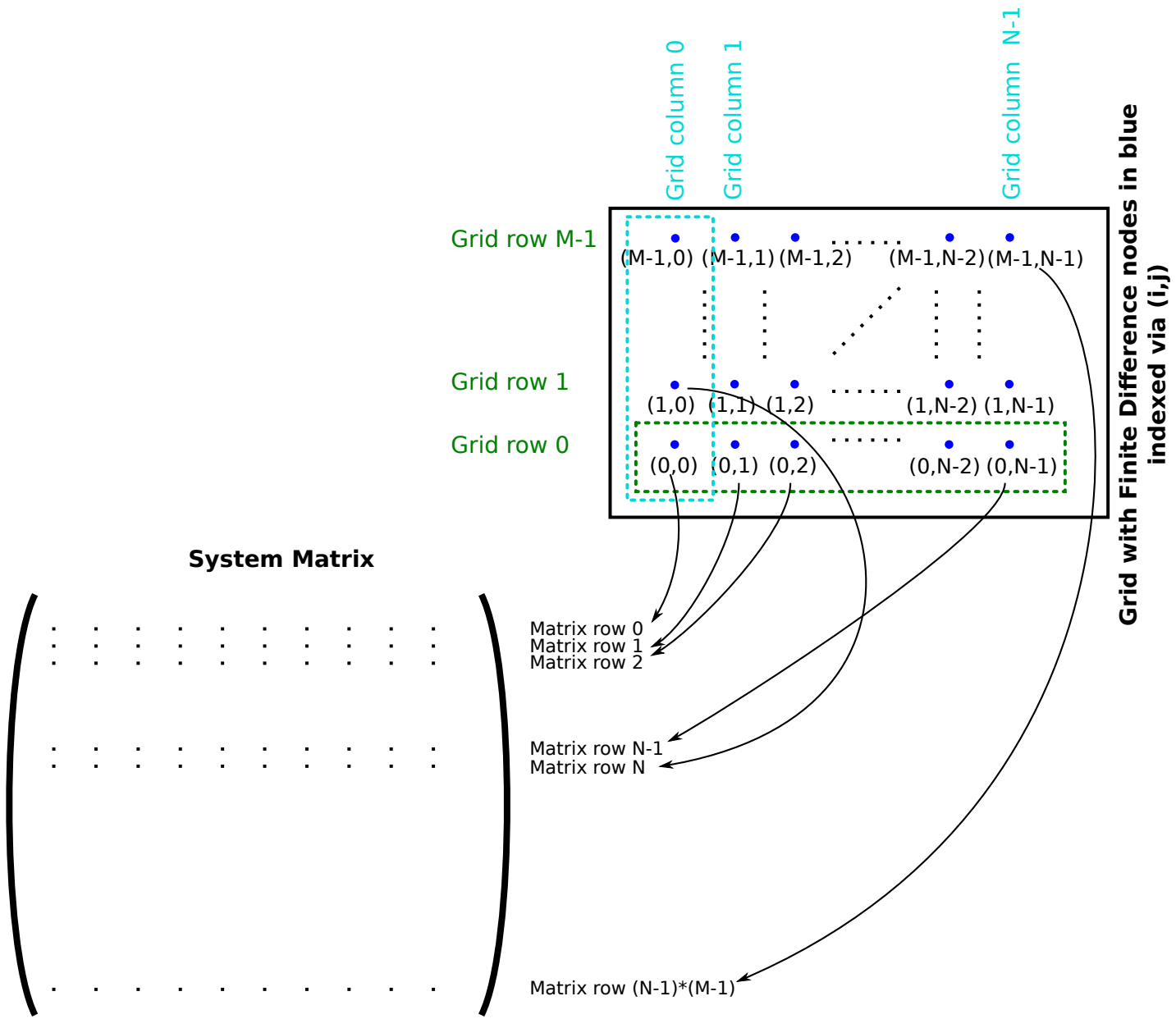
Step 3: Assembly for an $N \times M$ grid

```
__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];

      // diagonal entry
      col_indices[this_row_offset] = i * N + j;
      values[this_row_offset] = 4;
      this_row_offset += 1;

      if (i > 0) { // bottom neighbor
        col_indices[this_row_offset] = (i-1) * N + j;
        values[this_row_offset] = -1;
        this_row_offset += 1;
      }
      if (j > 0)   { /* similarly */ }
      if (i < N-1) { /* similarly */ }
      if (j < M-1) { /* similarly */ }
}   }
```

Finite Differences



Other Discretizations

Finite Volumes

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

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Finite Volumes

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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