AMATH 483/583
High Performance Scientific Computing

Lecture 9:
Strassen's Algorithm
Sparse Matrix Computation

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Overview

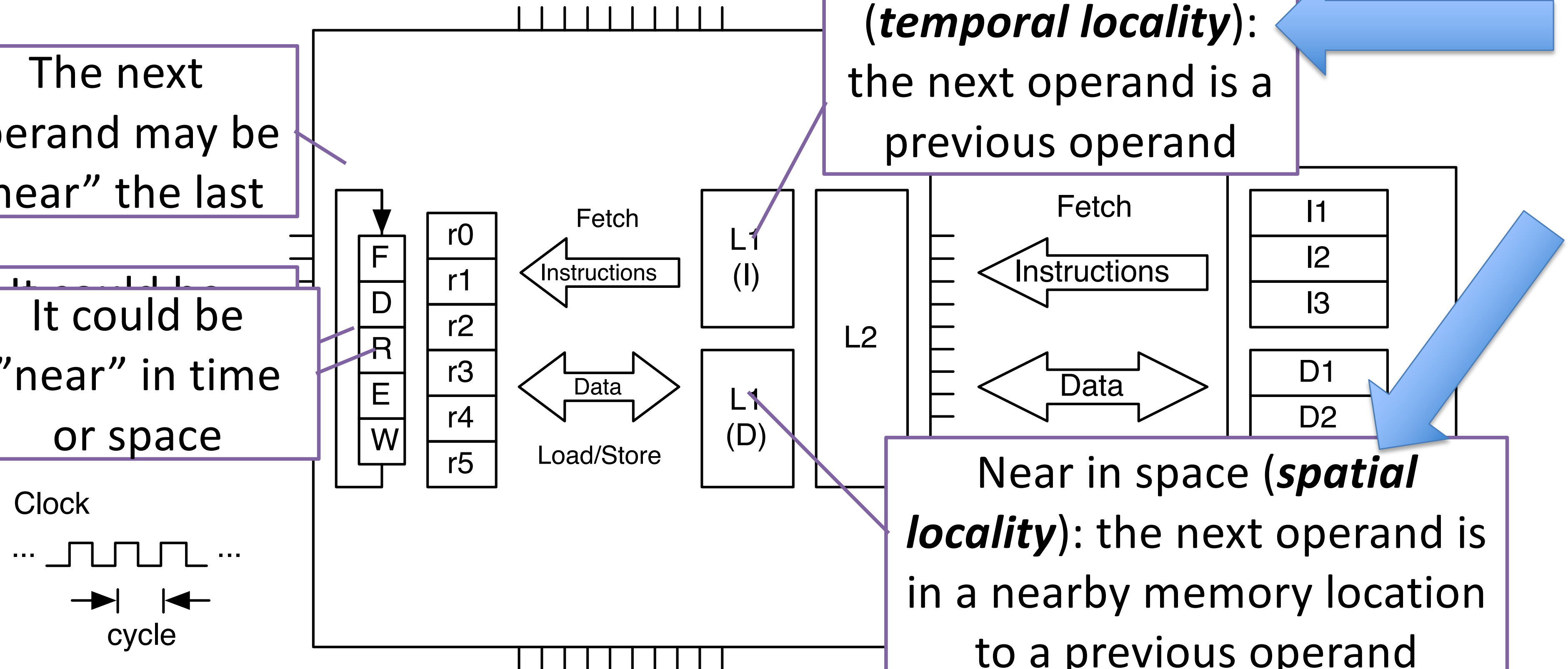
- Review: Locality and optimization strategies
- Sparsity
- Coordinate format (COO)
- Compressed sparse row (CSR)

Locality → Strategy

The next operand may be "near" the last

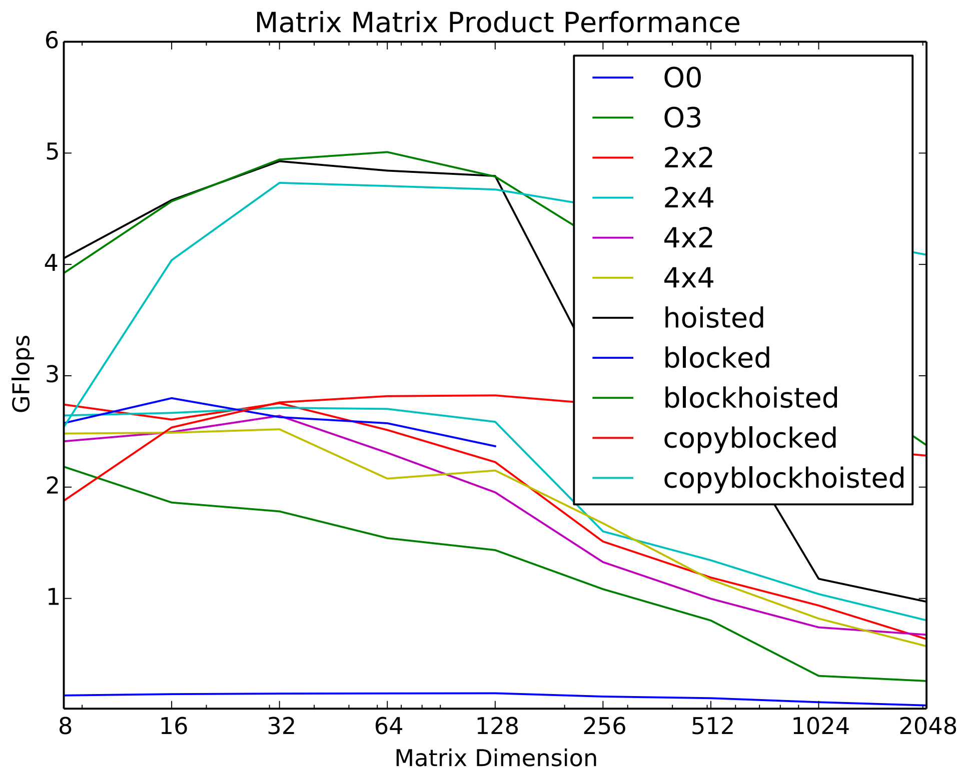
It could be "near" in time or space

Near in time (***temporal locality***): the next operand is a previous operand



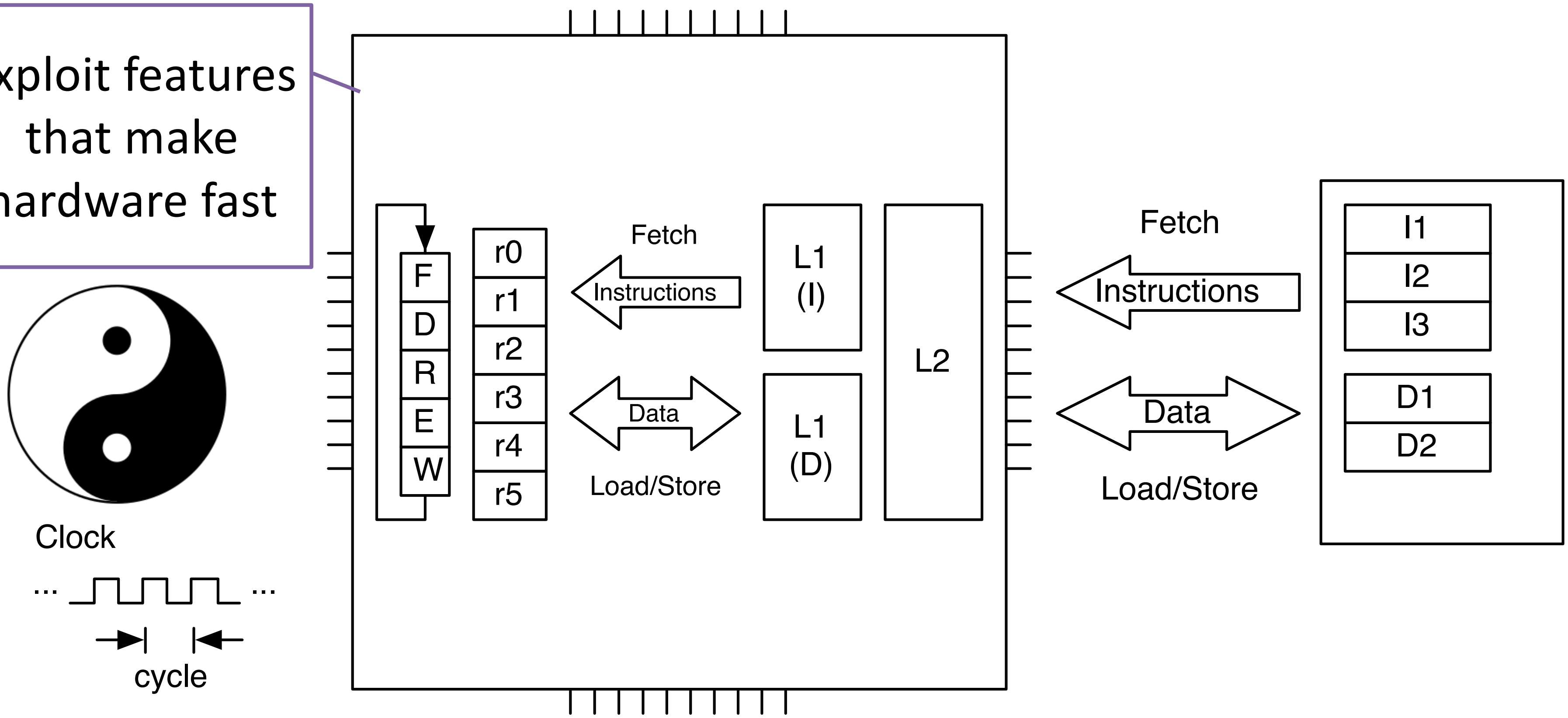
Near in space (***spatial locality***): the next operand is in a nearby memory location to a previous operand

Blocking and Tiling and Hoisting and Copying



What Else Can We Do for Performance

Exploit features that make hardware fast



General Performance Principles

- Work harder
  - Faster core
- Work smarter
  - Branch predictions, etc
  - Better compilation
  - Better algorithm
  - Better implementation
- Get help

Dennard scaling (ended 2005)

What about this?

We did this

Another Way to Work Smarter

(Work less)

Strassen's Algorithm

Volker Strassen.
Gaussian Elimination is not Optimal.
Numer Math, Vol 13, No.4, Aug 1969.

$$\begin{bmatrix} C_{00} & C_{01} \\ C_{10} & C_{11} \end{bmatrix} = \begin{bmatrix} A_{00} & A_{01} \\ A_{10} & A_{11} \end{bmatrix} \times \begin{bmatrix} B_{00} & B_{01} \\ B_{10} & B_{11} \end{bmatrix}$$

$$\begin{aligned} C_{00} &= A_{00}B_{00} + A_{01}B_{10} \\ C_{01} &= A_{00}B_{01} + A_{01}B_{11} \\ C_{10} &= A_{10}B_{00} + A_{11}B_{10} \\ C_{11} &= A_{10}B_{01} + A_{11}B_{11} \end{aligned}$$

Eight multiplies

If these are matrix blocks: Eight matrix multiplies

Strassen's Algorithm

$$\begin{bmatrix} C_{00} & C_{01} \\ C_{10} & C_{11} \end{bmatrix} = \begin{bmatrix} A_{00} & A_{01} \\ A_{10} & A_{11} \end{bmatrix} \times \begin{bmatrix} B_{00} & B_{01} \\ B_{10} & B_{11} \end{bmatrix}$$

Seven matrix multiplies

Recurse

$$\begin{aligned}
T_0 &= (A_{00} + A_{11})(B_{00} + B_{11}) \\
T_1 &= (A_{10} + A_{11})(B_{00}) \\
T_2 &= (A_{00})(B_{01} - B_{11}) \\
T_3 &= (A_{11})(B_{10} - B_{00}) \\
T_4 &= (A_{00} + A_{01})(B_{11}) \\
T_5 &= (A_{10} - A_{00})(B_{00} + B_{01}) \\
T_6 &= (A_{01} - A_{11})(B_{10} + B_{11})
\end{aligned}$$

Seven multiplies

Many adds and subtracts

$$\begin{aligned}
C_{00} &= T_0 + T_3 - T_4 + T_6 \\
C_{01} &= T_2 + T_4 \\
C_{10} &= T_1 + T_4 \\
C_{11} &= T_0 - T_1 + T_2 + T_5
\end{aligned}$$

Strassen's Algorithm

$$\begin{bmatrix} C_{00} & C_{01} \\ C_{10} & C_{11} \end{bmatrix} = \begin{bmatrix} A_{00} & A_{01} \\ A_{10} & A_{11} \end{bmatrix} \times \begin{bmatrix} B_{00} & B_{01} \\ B_{10} & B_{11} \end{bmatrix}$$

Seven matrix multiplies

Recurse

$$\begin{aligned}
T_0 &= (A_{00} + A_{11})(B_{00} + B_{11}) \\
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T_4 &= (A_{00} + A_{01})(B_{11}) \\
T_5 &= (A_{10} - A_{00})(B_{00} + B_{01}) \\
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\end{aligned}$$

$$\begin{aligned}
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C_{10} &= T_1 + T_4 \\
C_{11} &= T_0 - T_1 + T_2 + T_5
\end{aligned}$$

$$O(N^3) \text{ work vs } O(N^2) \text{ data}$$

Multiply

Add

Strassen's Algorithm

$$\begin{bmatrix} C_{00} & C_{01} \\ C_{10} & C_{11} \end{bmatrix} = \begin{bmatrix} A_{00} & A_{01} \\ A_{10} & A_{11} \end{bmatrix} \times \begin{bmatrix} B_{00} & B_{01} \\ B_{10} & B_{11} \end{bmatrix}$$

Divide and Conquer

$$\begin{aligned}
T_0 &= (A_{00} + A_{11})(B_{00} + B_{11}) \\
T_1 &= (A_{10} + A_{11})(B_{00}) \\
T_2 &= (A_{00})(B_{01} - B_{11}) \\
T_3 &= (A_{11})(B_{10} - B_{00}) \\
T_4 &= (A_{00} + A_{01})(B_{11}) \\
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\end{aligned}$$

$$\begin{aligned}
C_{00} &= T_0 + T_3 - T_4 + T_6 \\
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C_{10} &= T_1 + T_4 \\
C_{11} &= T_0 - T_1 + T_2 + T_5
\end{aligned}$$

Recurse

Seven matrix multiplies

$O(N^3)$ work vs $O(N^2)$ data

Each block is size $\frac{N}{2}$ → $\left(\frac{N}{2}\right)^3 = \frac{N^3}{8}$ → $\frac{7}{8}N^3$

Strassen's Algorithm

$$\begin{bmatrix} C_{00} & C_{01} \\ C_{10} & C_{11} \end{bmatrix} = \begin{bmatrix} A_{00} & A_{01} \\ A_{10} & A_{11} \end{bmatrix} \times \begin{bmatrix} B_{00} & B_{01} \\ B_{10} & B_{11} \end{bmatrix}$$

$$\frac{7}{8}\frac{7}{8}\cdots\frac{7}{8}$$

How many of these

Divide and conquer

$$\log_2(N)$$

$$\begin{aligned} T_0 &= (A_{00} + A_{11})(B_{00} + B_{11}) \\ T_1 &= (A_{10} + A_{11})(B_{00}) \\ T_2 &= (A_{00})(B_{01} - B_{11}) \\ T_3 &= (A_{11})(B_{10} - B_{00}) \\ T_4 &= (A_{00} + A_{01})(B_{11}) \\ T_5 &= (A_{10} - A_{00})(B_{00} + B_{01}) \\ T_6 &= (A_{01} - A_{11})(B_{10} + B_{11}) \end{aligned}$$

$$\begin{aligned} C_{00} &= T_0 + T_3 - T_4 + T_6 \\ C_{01} &= T_2 + T_4 \\ C_{10} &= T_1 + T_4 \\ C_{11} &= T_0 - T_1 + T_2 + T_5 \end{aligned}$$

$$O(N^{\log_2 7})$$

$$O(N^{\log_2 7}) \ll O(N^{\log_2 8}) = O(N^3)$$

Strassen's Algorithm

$$\begin{bmatrix} C_{00} & C_{01} \\ C_{10} & C_{11} \end{bmatrix} = \begin{bmatrix} A_{00} & A_{01} \\ A_{10} & A_{11} \end{bmatrix} \times \begin{bmatrix} B_{00} & B_{01} \\ B_{10} & B_{11} \end{bmatrix}$$

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T_5 &= (A_{10} - A_{00})(B_{00} + B_{01}) \\
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\end{aligned}$$

$$\begin{aligned}
C_{00} &= T_0 + T_3 - T_4 + T_6 \\
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C_{10} &= T_1 + T_4 \\
C_{11} &= T_0 - T_1 + T_2 + T_5
\end{aligned}$$

$O(N^{2.38})$

Better algorithms

Limit?

Require large N

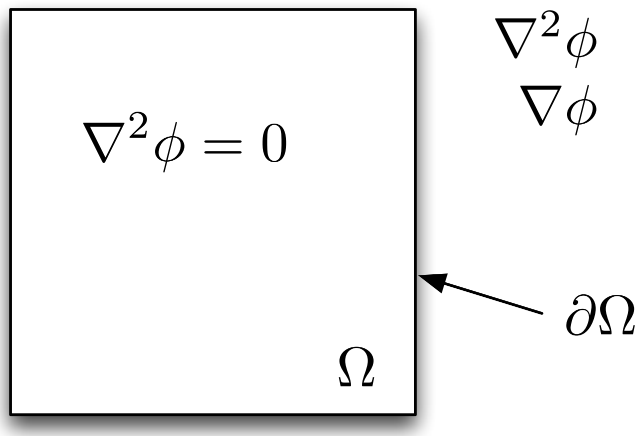
Limit Unknown, Biggest open question in numerical linear algebra

Another Way to Work Smarter

(Work less)

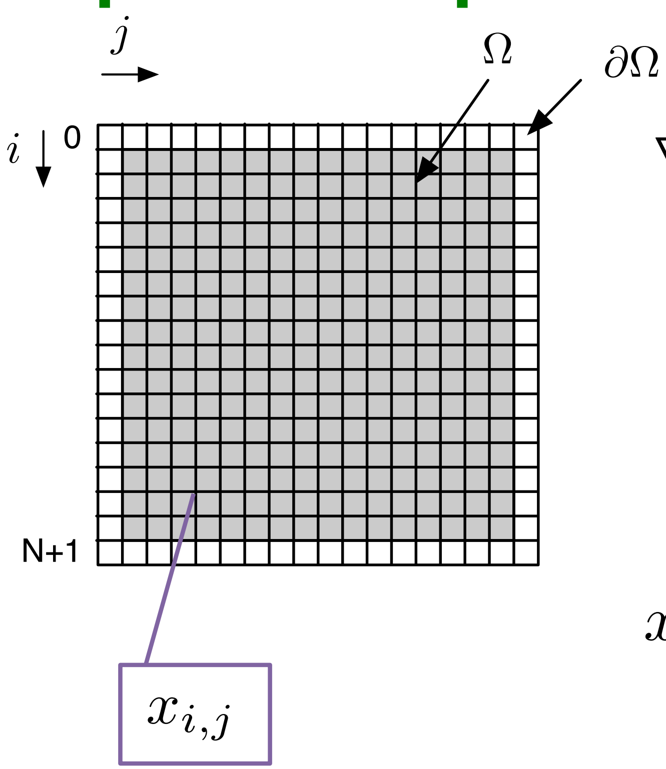
In Practice

- Many scientific applications are based on solving systems of partial differential equations that model physical phenomena
- Laplace's equation on unit square is prototypical PDE



$$\begin{aligned} \nabla^2\phi &= 0 \quad \text{on } \Omega \\ \nabla\phi &= f \quad \text{on } \partial\Omega \end{aligned}$$

Laplace's Equation on a Regular Grid



$$
\begin{aligned}
\nabla^2 \phi &= 0 \quad \text{on } \Omega \\
\phi &= f \quad \text{on } \partial\Omega
\end{aligned}
$$

Discretization

$$x_{i-1,j} + x_{i+1,j} + x_{i,j-1} + x_{i,j+1} - 4x_{i,j} = 0$$

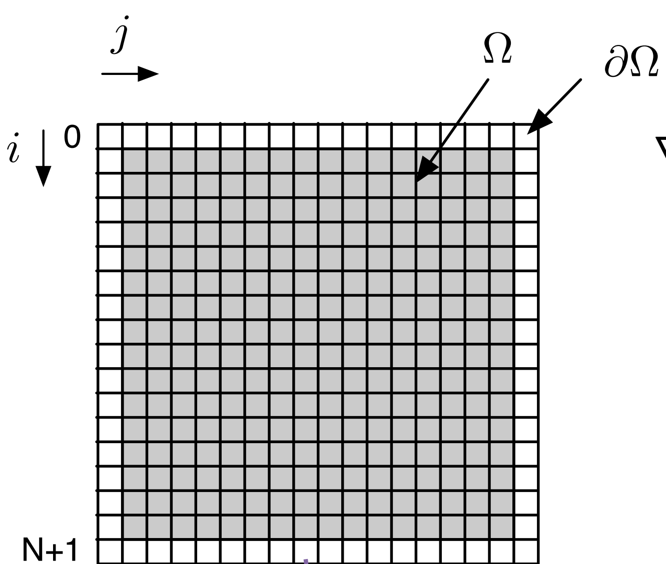
$$
\frac{1}{h^2}
\begin{bmatrix}
4 & -1 & \cdots & -1 & & \\
-1 & \ddots & \ddots & \ddots & \ddots & \\
\vdots & \ddots & \ddots & \ddots & \ddots & -1 \\
-1 & \ddots & \ddots & \ddots & \ddots & \vdots \\
 & \ddots & \ddots & \ddots & \ddots & -1 \\
 & & -1 & \cdots & -1 & 4
\end{bmatrix}
\begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ \vdots \\ \\ \end{bmatrix}
=
\begin{bmatrix} b_0 \\ b_1 \\ b_2 \\ \vdots \\ \\ \end{bmatrix}
$$

$$x_{i,j} = (x_{i-1,j} + x_{i+1,j} + x_{i,j-1} + x_{i,j+1})/4$$

The value of each point on the grid

The average of its neighbors

Laplace's Equation on a Regular Grid



Why isn't 0 the solution?

$$\begin{aligned} \nabla^2\phi &= 0 \quad \text{on } \Omega \\ \phi &= f \quad \text{on } \partial\Omega \end{aligned}$$

The boundary is non-zero

Discret

$$\frac{1}{h^2}\begin{bmatrix} 4 & -1 & \cdots & -1 & & \\ -1 & \ddots & \ddots & \ddots & \ddots & \\ \vdots & \ddots & \ddots & \ddots & \ddots & -1 \\ -1 & \ddots & \ddots & \ddots & \ddots & \vdots \\ & \ddots & \ddots & \ddots & \ddots & -1 \\ & & -1 & \cdots & -1 & 4 \end{bmatrix} \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ \vdots \\ \\ \end{bmatrix} = \begin{bmatrix} b_0 \\ b_1 \\ b_2 \\ \vdots \\ \\ \end{bmatrix}$$

Non-zeros in here due to boundary

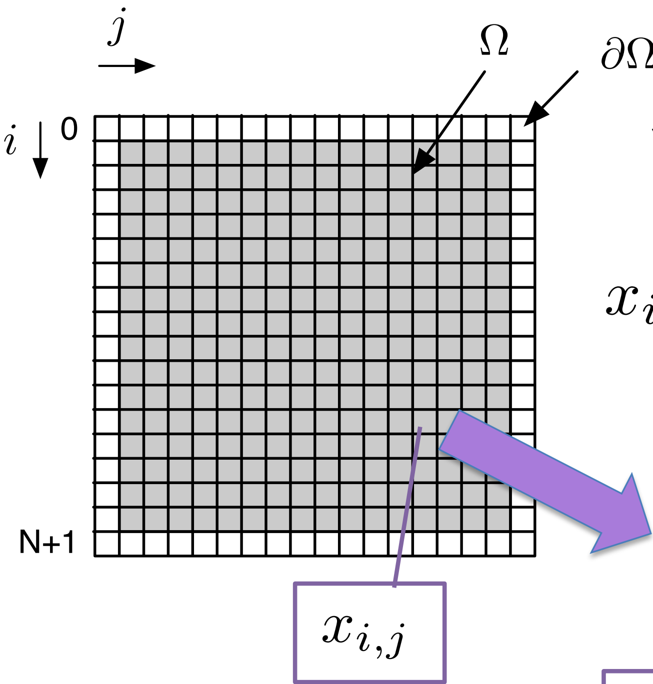
$$x_{i,j} = (x_{i-1,j} + x_{i+1,j} + x_{i,j-1} + x_{i,j+1})/4$$

The boundary is non-zero

The value of each point on the grid

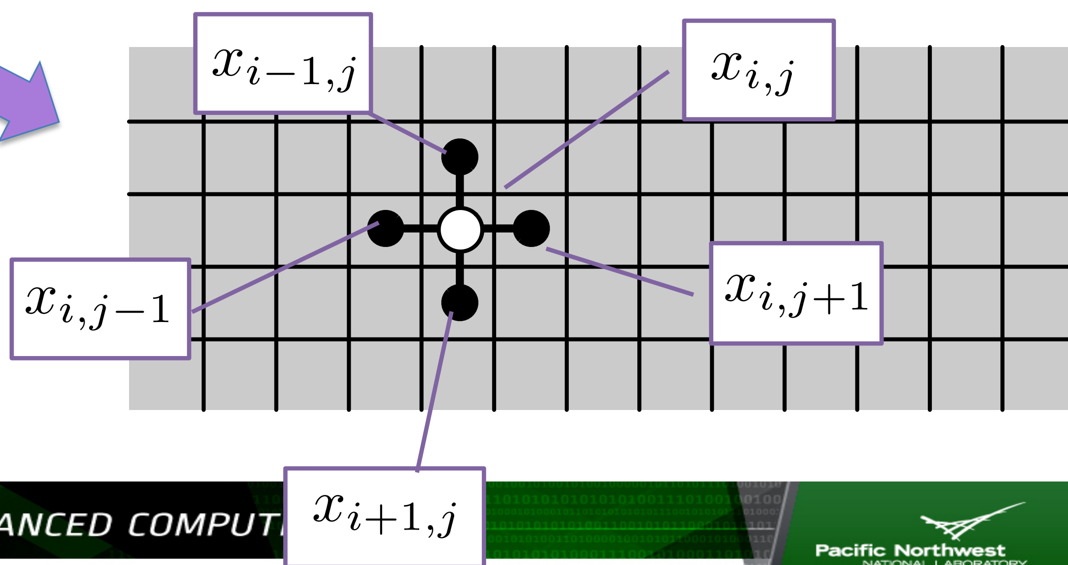
The average of its neighbors

Laplace's Equation on a Regular Grid

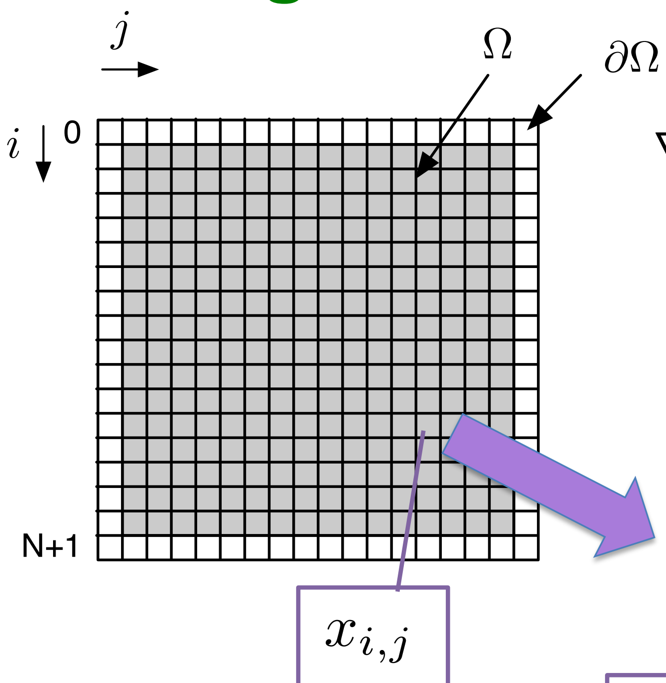


$$
\begin{aligned}
\nabla^2 \phi &= 0 \quad \text{on } \Omega \\
\phi &= f \quad \text{on } \partial\Omega
\end{aligned}
$$

$$x_{i,j} = (x_{i-1,j} + x_{i+1,j} + x_{i,j-1} + x_{i,j+1})/4$$



Iterating for a solution

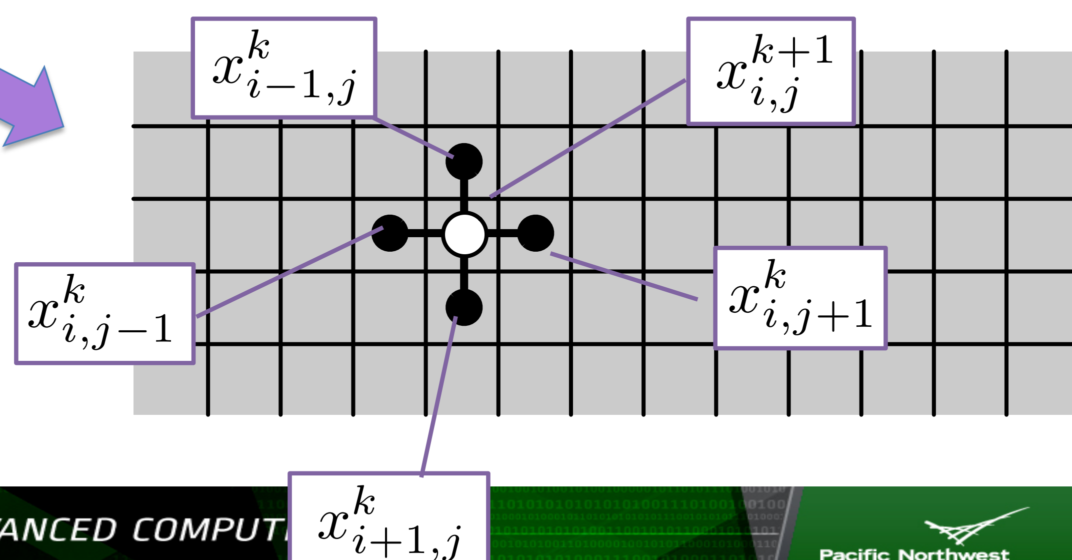


$$\nabla^2\phi = 0 \quad \text{on } \Omega$$
$$\phi = f \quad \text{on } \partial\Omega$$

Approximation at iteration k+1

Average of approximation at iteration k

$$x_{i,j}^{k+1} = (x_{i-1,j}^{k} + x_{i+1,j}^{k} + x_{i,j-1}^{k} + x_{i,j+1}^{k})/4$$



Iterating for a soluti

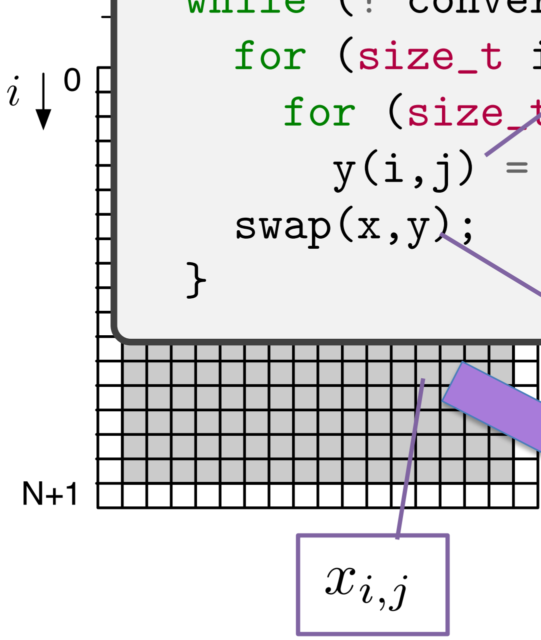
```
while (! converged()) {
  for (size_t i = 1; i < N+1; ++i)
    for (size_t j = 1; j < N+1; ++j)
      y(i,j) = (x(i-1,j) + x(i+1,j) + x(i,j-
  swap(x,y);
}
```

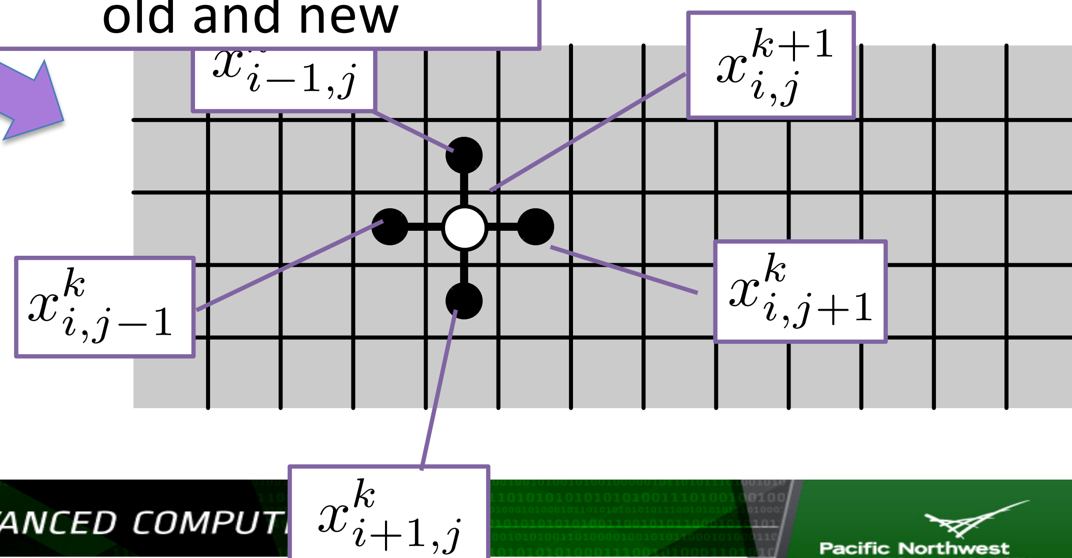
Approximation at iteration k+1

Average of approximation at iteration k

At end of each outer iteration: new becomes old (and v.v.)

Only need to use two arrays to do iteration: old and new

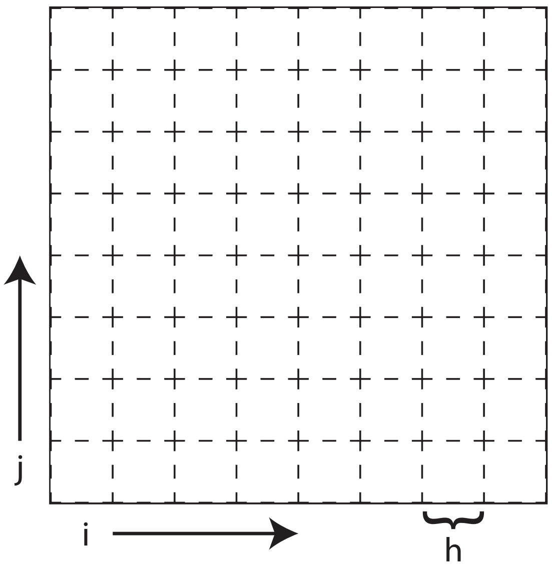




Discretized

- Del operator

$$\nabla\phi = \frac{\partial\phi}{\partial x} + \frac{\partial\phi}{\partial y}$$
$$\nabla^2\phi = \frac{\partial^2\phi}{\partial x^2} + \frac{\partial^2\phi}{\partial y^2}$$



- Finite difference approximation to derivative

$$\begin{aligned}
\frac{\mathrm{d}x}{\mathrm{d}t}(t_0) &\approx \frac{x(t_0+h)-x(t_0)}{h}\\
\frac{\mathrm{d}^2x}{\mathrm{d}t^2}(t_0) &\approx \frac{\frac{\mathrm{d}x}{\mathrm{d}t}(t_0+h)-\frac{\mathrm{d}x}{\mathrm{d}t}(t_0)}{h}\\
&= \frac{x(t_0+h+h)-x(t_0+h)-x(t_0+h)+x(t_0)}{h^2}\\
&= \frac{x(t_0+2h)-2x(t_0+h)+x(t_0)}{h^2}\\
&= \frac{x(t_0+h)-2x(t_0)+x(t_0-h)}{h^2}
\end{aligned}$$

- Finite difference approximation to del

$$\frac{\phi_{i+1,j} + \phi_{i-1,j} + \phi_{i,j-1} + \phi_{i,j+1} - 4\phi_{i,k}}{h^2} = 0$$

Matrix Formulation

- Lexicographically order unknowns (note some will be boundary values)

$$\frac{x_{i+1} + x_{i-1} + x_{i+N} + x_{i-N} - 4x_i}{h^2} = 0$$

- Formulate as a matrix problem:

$$\frac{1}{h^2}\begin{bmatrix} 4 & -1 & \cdots & -1 & & \\ -1 & \ddots & \ddots & \ddots & \ddots & \\ \vdots & \ddots & \ddots & \ddots & \ddots & -1 \\ -1 & \ddots & \ddots & \ddots & \ddots & \vdots \\ & \ddots & \ddots & \ddots & \ddots & -1 \\ & & -1 & \cdots & -1 & 4 \end{bmatrix} \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ \vdots \\ \\ \\ \end{bmatrix} = \begin{bmatrix} b_0 \\ b_1 \\ b_2 \\ \vdots \\ \\ \\ \end{bmatrix}$$

Linear System Solution

```
void multiply(const Matrix& A, const Matrix& B, Ma
  for (size_t i = 0; i < A.num_rows(); ++i) {
    for (size_t j = 0; j < B.num_cols(); ++j) {
      for (size_t k = 0; k < A.num_cols(); ++k) {
        C(i, j) += A(i, k) * B(k, j);
      }
    }
  }
}
```

Matrix-matrix product is kernel operation

What happens with the Laplacian matrix?

Multiplying and adding zero to zero

Work Smarter! Don’t multiply and add zero to zero

Solution?

```
void multiply(const Matrix& A, const Matrix& B, Matrix& C) {
  for (size_t i = 0; i < A.num_rows(); ++i) {
    for (size_t j = 0; j < B.num_cols(); ++j) {
      for (size_t k = 0; k < A.num_cols(); ++k) {
        if(A(i,k) != 0.0 && B(k,j) != 0) {
          C(i, j) += A(i, k) * B(k, j);
        }
      }
    }
  }
}
```

Avoid zeros

But we still touch every element

And that's what expensive

Solution?

```
void multiply(const Matrix& A, const Matrix& B, Matrix& C) {
  for (size_t i = 0; i < A.num_rows(); ++i) {
    for (size_t j = 0; j < B.num_cols(); ++j) {
      for (size_t k = 0; k < A.num_cols(); ++k) {
        if(A(i,k) != 0.0 && B(k,j) != 0) {
          C(i, j) += A(i, k) * B(k, j);
        }
      }
    }
  }
}
```

We need to avoid zeros

Without looking to see if there is a zero

Solution: Sparse Matrices

In order to avoid zeros

Don't store zeros

A zero is a null op

Use data structures and algorithms accordingly

Sparse matrix techniques

$$\frac{1}{h^2}\begin{bmatrix} 4 & -1 & \cdots & -1 & & \\ -1 & \ddots & \ddots & \ddots & \ddots & \\ \vdots & \ddots & \ddots & \ddots & \ddots & -1 \\ -1 & \ddots & \ddots & \ddots & \ddots & \vdots \\ & \ddots & \ddots & \ddots & \ddots & -1 \\ & & -1 & \cdots & -1 & 4 \end{bmatrix} \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ \vdots \\ \\ \\ \end{bmatrix} = \begin{bmatrix} b_0 \\ b_1 \\ b_2 \\ \vdots \\ \\ \\ \end{bmatrix}$$

Solving Sparse Systems

- Work only with non-zeros
- Direct methods
  - Perform LU factorization on sparse matrix
  - Create non-zeros during elimination process
  - Pre-order (using heuristics) to minimize the amount of fill
  - Very sequential
  - Fill can be quite significant
- Iterative methods
  - Successively create better approximations to x
  - Relaxation methods (e.g., Jacobi) – very very very slow to converge
  - Krylov subspace methods (e.g., conjugate gradient)
    - Good preconditioning often required

$$\frac{1}{h^2}\begin{bmatrix} 4 & -1 & \cdots & -1 & & \\ -1 & \ddots & \ddots & \ddots & \ddots & \\ \vdots & \ddots & \ddots & \ddots & \ddots & -1 \\ -1 & \ddots & \ddots & \ddots & \ddots & \vdots \\ & \ddots & \ddots & \ddots & \ddots & -1 \\ & & -1 & \cdots & -1 & 4 \end{bmatrix} \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ \vdots \\ \\ \\ \end{bmatrix} = \begin{bmatrix} b_0 \\ b_1 \\ b_2 \\ \vdots \\ \\ \\ \end{bmatrix}$$

A zero here

Turns into a non-zero

Need to create new space (fill)

Conjugate Gradient Algorithm

Initial $r^{(0)}=b-Ax^{(0)}$

For i=1, 2, …

  solve $Mz^{(i-1)} = r^{(i-1)}$

  $\rho_{i-1} = r^{(i-1)T} z^{(i-1)}$

  If i=1

    $p^{(1)} = z^{(0)}$

  Else

    $\beta_{i-1} = \rho_{i-1} / \rho_{i-2}$

    $p^{(i)} = z^{(i-1)} + \beta_{i-1} p^{(i-1)}$

  Endif

  $q^{(i)} = Ap^{(i)}$

  $\alpha_i = \rho_{i-1} / p^{(i)T} q^{(i)}$

  $x^{(i)} = x^{(i-1)} + \alpha_i p^{(i)}$

  $r^{(i)} = r^{(i-1)} - \alpha_i q^{(i)}$

  Check convergence

end

```
mult(A, scaled(x, -1.0), b, r);
while (! iter.finished(r)) {
  solve(M, r, z);
  rho = dot_conj(r, z);

  if ( iter.first() )
    copy(z, p);
  else {
    beta = rho / rho_1;
    add(z, scaled(p, beta), p);
  }
  mult(A, p, q);
  alpha = rho / dot_conj(p, q);
  add(x, scaled(p, alpha), x);
  add(r, scaled(q, -alpha), r);
  rho_1 = rho;
  ++iter;
}
```

Key operation

Sparse Storage

- A matrix is map from two indices to a value

$$\frac{1}{h^2}\begin{bmatrix} 4 & -1 & \cdots & -1 & & \\ -1 & \ddots & \ddots & \ddots & \ddots & \\ \vdots & \ddots & \ddots & \ddots & \ddots & -1 \\ -1 & \ddots & \ddots & \ddots & \ddots & \vdots \\ & \ddots & \ddots & \ddots & \ddots & -1 \\ & & -1 & \cdots & -1 & 4 \end{bmatrix} \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ \vdots \\ \\ \\ \end{bmatrix} = \begin{bmatrix} b_0 \\ b_1 \\ b_2 \\ \vdots \\ \\ \\ \end{bmatrix}$$

- So if we want to store just elements that are not zero (the “non-zeros”)
- We need to store the two indices and the value

Dense Storage

$$\begin{bmatrix} 3 & 0 & 0 & 8 & 0 & 0 \\ 0 & 1 & 4 & 0 & 6 & 0 \\ 0 & 0 & 0 & 0 & 0 & 7 \\ 5 & 0 & 4 & 1 & 0 & 0 \\ 0 & 3 & 0 & 0 & 5 & 0 \\ 0 & 0 & 0 & 0 & 0 & 9 \end{bmatrix}$$

Dense storage: all matrix elements are kept

At location corresponding to indices

3	0	0	8	0	0	0	1	4	0	6	0	0	0	0	0	0	7	5	0	4	1	0	0	0	3	0	0	5	0	0

Matrix-Vector Product

$$\begin{bmatrix} 3 & 0 & 0 & 8 & 0 & 0 \\ 0 & 1 & 4 & 0 & 6 & 0 \\ 0 & 0 & 0 & 0 & 0 & 7 \\ 5 & 0 & 4 & 1 & 0 & 0 \\ 0 & 3 & 0 & 0 & 5 & 0 \\ 0 & 0 & 0 & 0 & 0 & 9 \end{bmatrix}$$

```
void matvec(const Matrix& A, const Vector& x, const Vector& y) }
  for (size_t i = 0; i < A.num_rows(); ++i) {
    for (size_t j = 0; j < A.num_cols(); ++j) {
      y(i) += A(i, j) * x(j);
    }
  }
}
```

And thus all values of A

Zeros and non-zeros

We go through all possible valid indices

3	0	0	8	0	0	0	1	4	0	6	0	0	0	0	0	0	7	5	0	4	1	0	0	0	3	0	0	5	0	0

Matrix-Vector Product

$$\begin{bmatrix} 3 & 0 & 0 & 8 & 0 & 0 \\ 0 & 1 & 4 & 0 & 6 & 0 \\ 0 & 0 & 0 & 0 & 0 & 7 \\ 5 & 0 & 4 & 1 & 0 & 0 \\ 0 & 3 & 0 & 0 & 5 & 0 \\ 0 & 0 & 0 & 0 & 0 & 9 \end{bmatrix}$$

```
void matvec(const Matrix& A, const Vector& x, const Vector& y) }
  for (size_t i = 0; i < A.num_rows(); ++i) {
    for (size_t j = 0; j < A.num_cols(); ++j) {
      y(i) += A(i, j) * x(j);
    }
  }
```

And row index

Need value of matrix entry

And column index

3	0	0	8	0	0	0	1	4	0	6	0	0	0	0	0	0	7	5	0	4	1	0	0	0	3	0	0	5	0	0

OK. We've stored all values

With dense storage, we loop through all possible indices and look up corresponding value

Sparse Storage

$$\begin{bmatrix} 3 & 0 & 0 & 8 & 0 & 0 \\ 0 & 1 & 4 & 0 & 6 & 0 \\ 0 & 0 & 0 & 0 & 0 & 7 \\ 5 & 0 & 4 & 1 & 0 & 0 \\ 0 & 3 & 0 & 0 & 5 & 0 \\ 0 & 0 & 0 & 0 & 0 & 9 \end{bmatrix}$$

```
void matvec(const Matrix& A, const Vector& x, const Vector& y) }
  for (size_t i = 0; i < A.num_rows(); ++i) {
    for (size_t j = 0; j < A.num_cols(); ++j) {
      y(i) += A(i, j) * x(j);
    }
  }
}
```

Goal: Loop over all indices for non-zero entries

3	8	1	4	6	7	5	4	1	3	5	9

So we need to store indices also

Store only the non-zeros

But what is non-zero is a property of matrix

Algorithm can't know it

Sparse Storage

$(0,0)$ $(0,3)$

$$\begin{bmatrix} 3 & 0 & 0 & 8 & 0 & 0 \\ 0 & 1 & 4 & 0 & 6 & 0 \\ 0 & 0 & 0 & 0 & 0 & 7 \\ 5 & 0 & 4 & 1 & 0 & 0 \\ 0 & 3 & 0 & 0 & 5 & 0 \\ 0 & 0 & 0 & 0 & 0 & 9 \end{bmatrix}$$

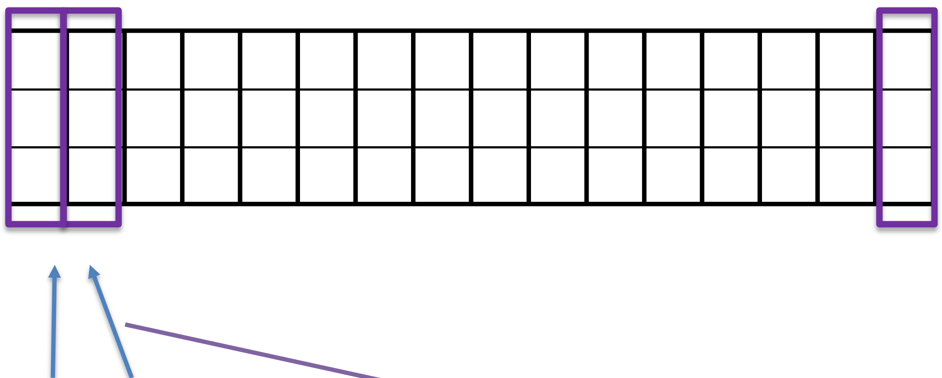
```
void matvec(const Matrix& A, const Vector& x, const Vector& y) }
  for (size_t i = 0; i < A.num_rows(); ++i) {
    for (size_t j = 0; j < A.num_cols(); ++j) {
      y(i) += A(i, j) * x(j);
    }
  }
}
```

Goal: Loop over all indices for non-zero entries

3	8	1	4	6	7	5	4	1	3	5	9
0	0	1	1	1	2	3	3	3	4	4	5
0	3	1	2	4	5	0	2	3	1	4	5

Does order of elements matter?

Coordinate Storage (Array of Structs)



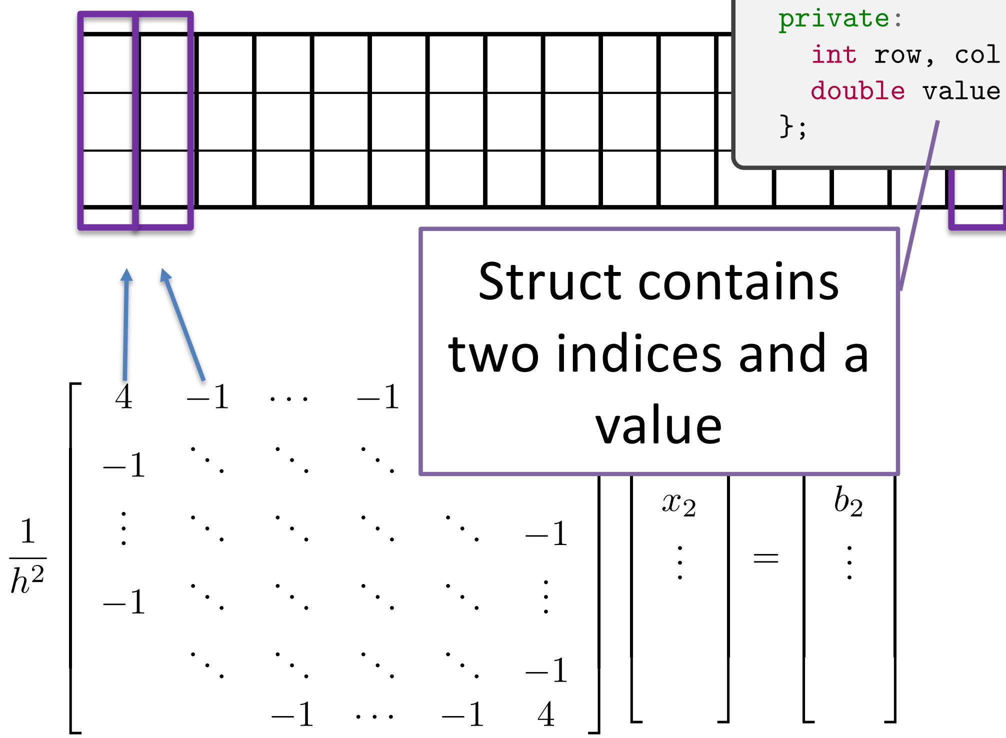
Single array with 3-element structs

Struct contains two indices and a value

Each element has two indices and a value stored

$$\frac{1}{h^2}\begin{bmatrix} 4 & -1 & \cdots & -1 & & \\ -1 & \ddots & \ddots & \ddots & \ddots & \\ \vdots & \ddots & \ddots & \ddots & \ddots & -1 \\ -1 & \ddots & \ddots & \ddots & \ddots & \vdots \\ & \ddots & \ddots & \ddots & \ddots & -1 \\ & & -1 & \cdots & -1 & 4 \end{bmatrix} \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ \vdots \\ \\ \\ \end{bmatrix} = \begin{bmatrix} b_0 \\ b_1 \\ b_2 \\ \vdots \\ \\ \\ \end{bmatrix}$$

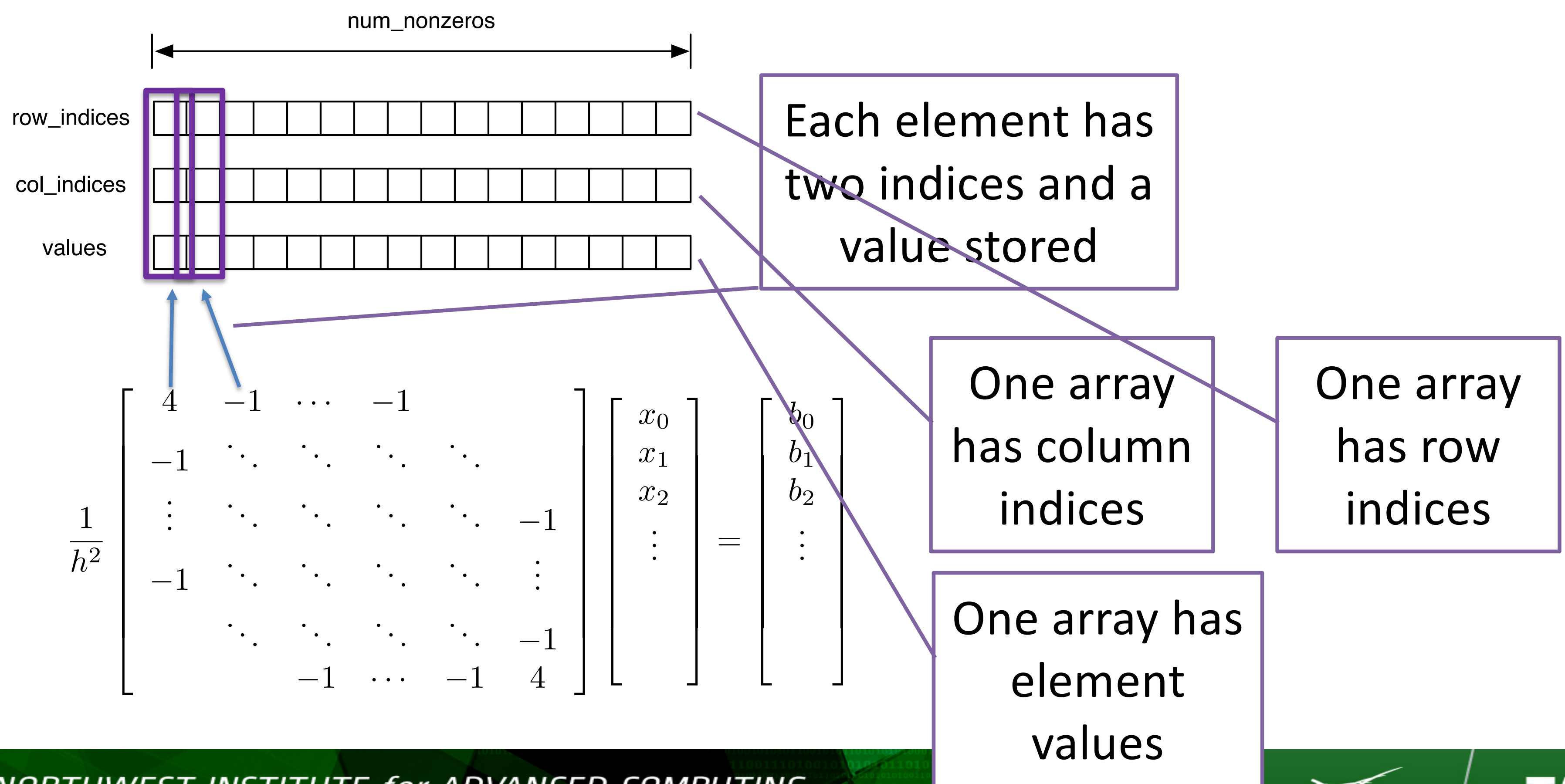
Coordinate Storage (Array of Structs)



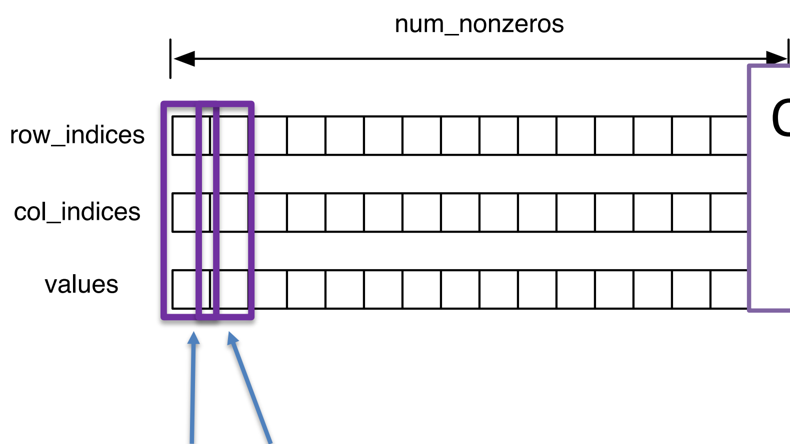

```
struct Element {
private:
  int row, col;
  double value;
};
```

```
struct COOMatrix {
private:
  std::vector<Element> arrayData;
};
```

Coordinate Storage (Struct of Arrays)



Coordinate Storage (Struct of Arrays)



One array has element values

```
struct COOMatrix {
private:
  std::vector<size_t> row_indices_;
  std::vector<size_t> col_indices_;
  std::vector<double> values_;
};
```

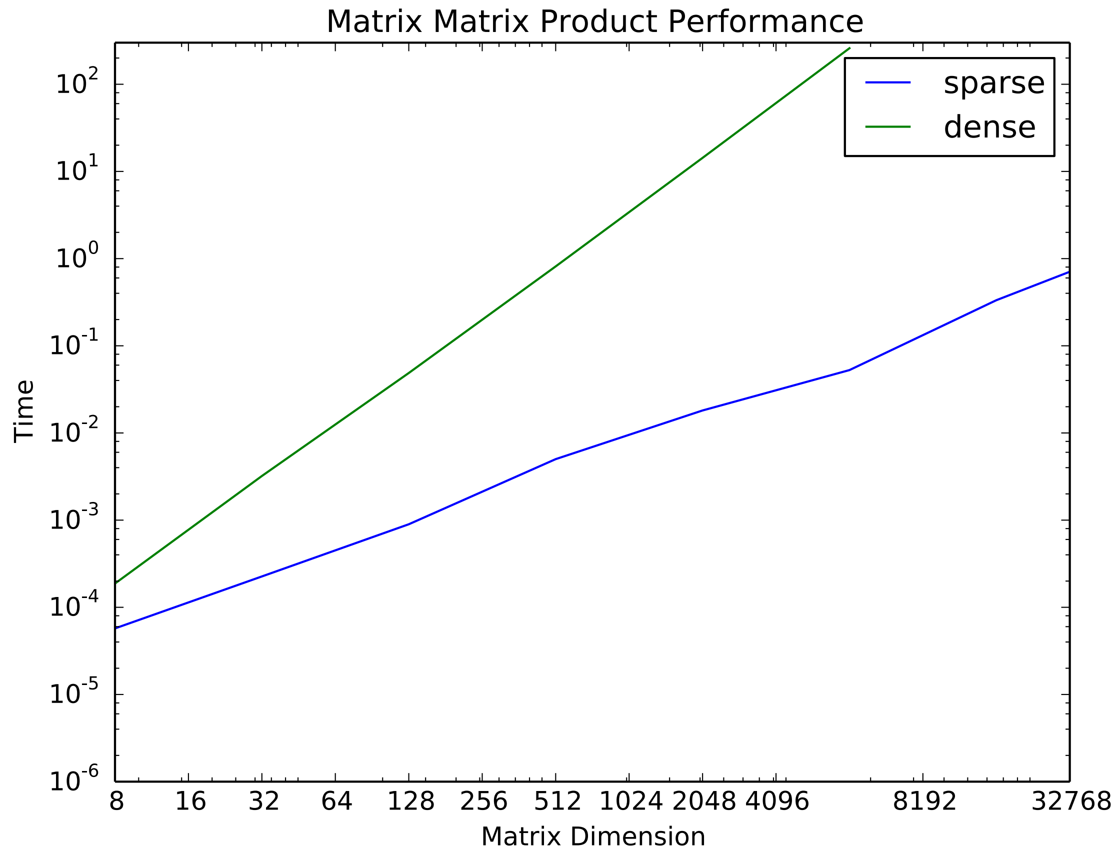
$$\frac{1}{h^2}\begin{bmatrix} 4 & -1 & \cdots & -1 & & & \\ -1 & \ddots & \ddots & \ddots & \ddots & & \\ \vdots & \ddots & \ddots & \ddots & \ddots & -1 \\ -1 & \ddots & \ddots & \ddots & \ddots & \vdots \\ & \ddots & \ddots & \ddots & \ddots & -1 \\ & & -1 & \cdots & -1 & 4 \end{bmatrix} \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ \vdots \\ \\ \\ \end{bmatrix} = \begin{bmatrix} b_0 \\ b_1 \\ b_2 \\ \vdots \\ \\ \\ \end{bmatrix}$$

One array has column indices

One array has row indices

Conventional Wisdom: Struct of Arrays is faster

Performance Comparison



What's the Catch?

In fact, it's a reference, so we can modify it

```
class Matrix {
public:
  Matrix(size_t M, size_t N) : num_rows_(M), num_cols_(N), storage_(num_rows_ * num_cols_) {}

        double& operator()(size_t i, size_t j)       { return storage_[i * num_cols_ + j]; }
  const double& operator()(size_t i, size_t j) const { return storage_[i * num_cols_ + j]; }

  size_t num_rows() const { return num_rows_; }
  size_t num_cols() const { return num_cols_; }

private:
  size_t              num_rows_, num_cols_;
  std::vector<double> storage_;
};
```

Provide indices, get back value

In constant time

Uh…

```
class COOMatrix {
public:
  COOMatrix(size_t M, size_t N) : num_rows_(M),

  size_t num_rows()     const { return num_rows_; }
  size_t num_cols()     const { return num_cols_; }

private:
  size_t num_rows_, num_cols_;
  std::vector<size_t> row_indices_, col_indices_;
  std::vector<double> storage_;
};
```

How do we get to a value (in constant time)?

We can't

Next Problem

```
void matvec(const Matrix& A, const Vector& x, Vector& y) {
  for (size_t i = 0; i < A.num_rows(); ++i) {
    for (size_t j = 0; j < A.num_cols(); ++j) {
      y(i) += A(i, j) * x(j);
    }
  }
}
```

Nice external function using operator()()

```
void matvec(const COOMatrix& A, const Vector& x, Vector& y) {
 // ??
}
```

No operator()() no external function

Coordinate Matvec

```
void matvec(const Matrix& A, const Vector& x, Vector& y) {
  for (size_t i = 0; i < A.num_rows(); ++i) {
    for (size_t j = 0; j < A.num_cols(); ++j) {
      y(i) += A(i, j) * x(j);
    }
  }
}
```

This is the row index

This is the value

This is the column index

Coordinate Matvec

```
void matvec(const Matrix& A, const Vector& x, Vector& y) {
  for (size_t i = 0; i < A.num_rows(); ++i) {
    for (size_t j = 0; j < A.num_cols(); ++j) {
      y(i) = A(i, j) * x(j);
    }
  }
}
```

Index into y with row index

Multiply by the corresponding value

Index into x with column index

We have these three things in coordinate format

Coordinate Matrix Mat Vec

```
class COOMatrix {
public:
  COOMatrix(size_t M, size_t N) : num_rows_(M), num_cols_(N)

  void matvec(const Vector& x, Vector& y) const {
    for (size_t k = 0; k < storage_.size(); ++k) {
      y(row_indices_[k]) += storage_[k] * x(col_indices[k]);
    }
  }

private:
  int num
  std::ve              _indic
  std::ve              rage_;
};
```

Meditate on this

Index into y with row index

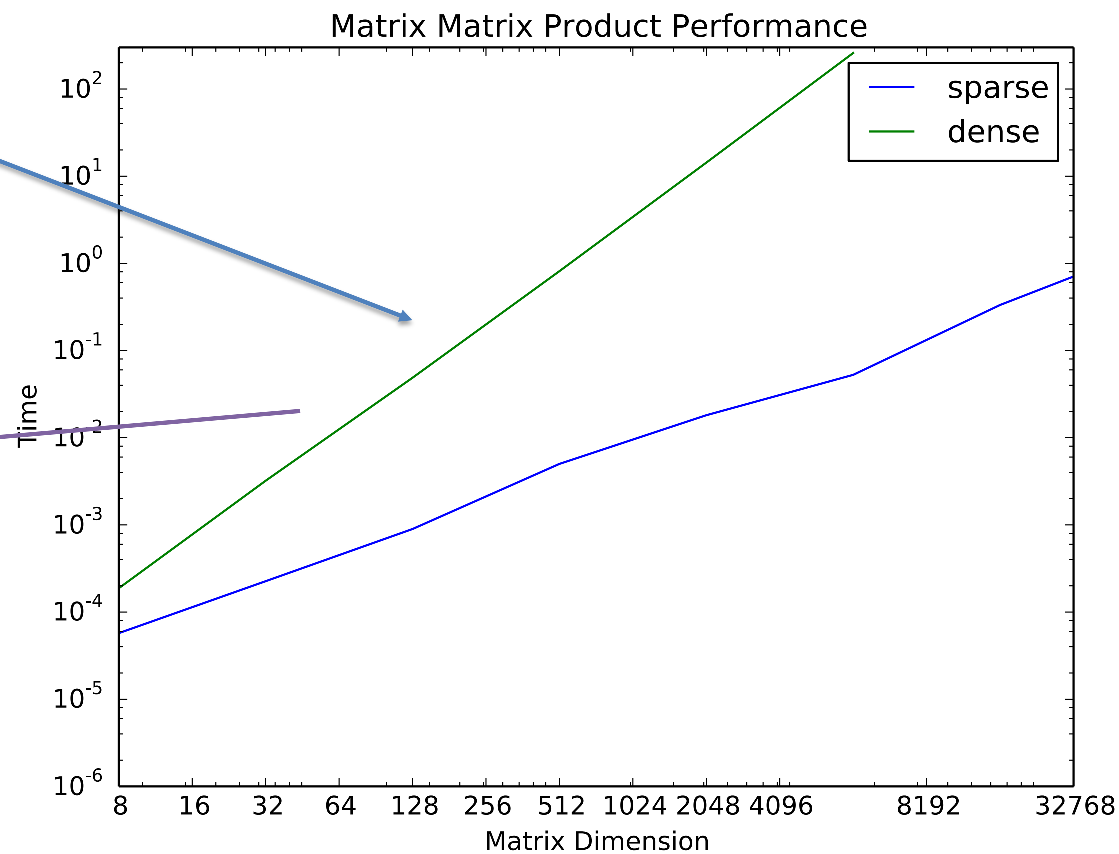
Multiply by corresponding value

Index into x with column index

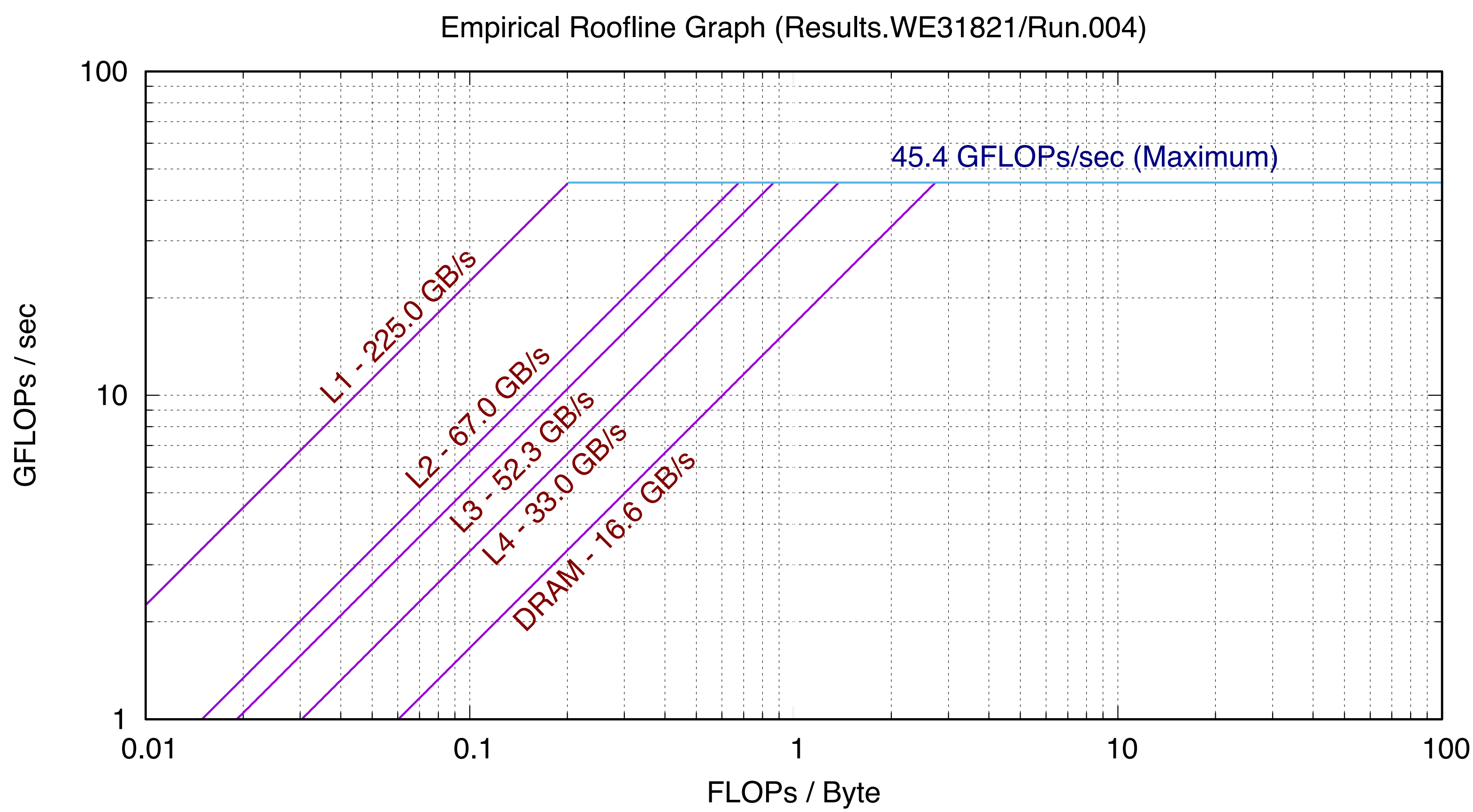
Performance Comparison

$O(N^3)$

10X problem size = 1000X run time



Roofline


Empirical Roofline Graph (Results.WE31821/Run.004)
GFLOPs / sec
FLOPs / Byte
100
10
1
0.01
0.1
1
10
100
45.4 GFLOPs/sec (Maximum)
L1 - 225.0 GB/s
L2 - 67.0 GB/s
L3 - 52.3 GB/s
L4 - 33.0 GB/s
DRAM - 16.6 GB/s

Numerical Intensity

```
void matvec(const Vector& x, Vector& y) const {
  for (size_type k = 0; k < arrayData.size(); ++k) {
    y(rowIndices[k]) += arrayData[k] * x(rowIndices[k]);
  }
}
```

Three doubles + 2 ints
= 32 bytes? (36 bytes?)

Two flops

5N

NNZ doubles
$+2$ NNZ indexes
$+2N$ doubles

$\frac{1}{14}\ \frac{\text{Flop}}{\text{byte}}$

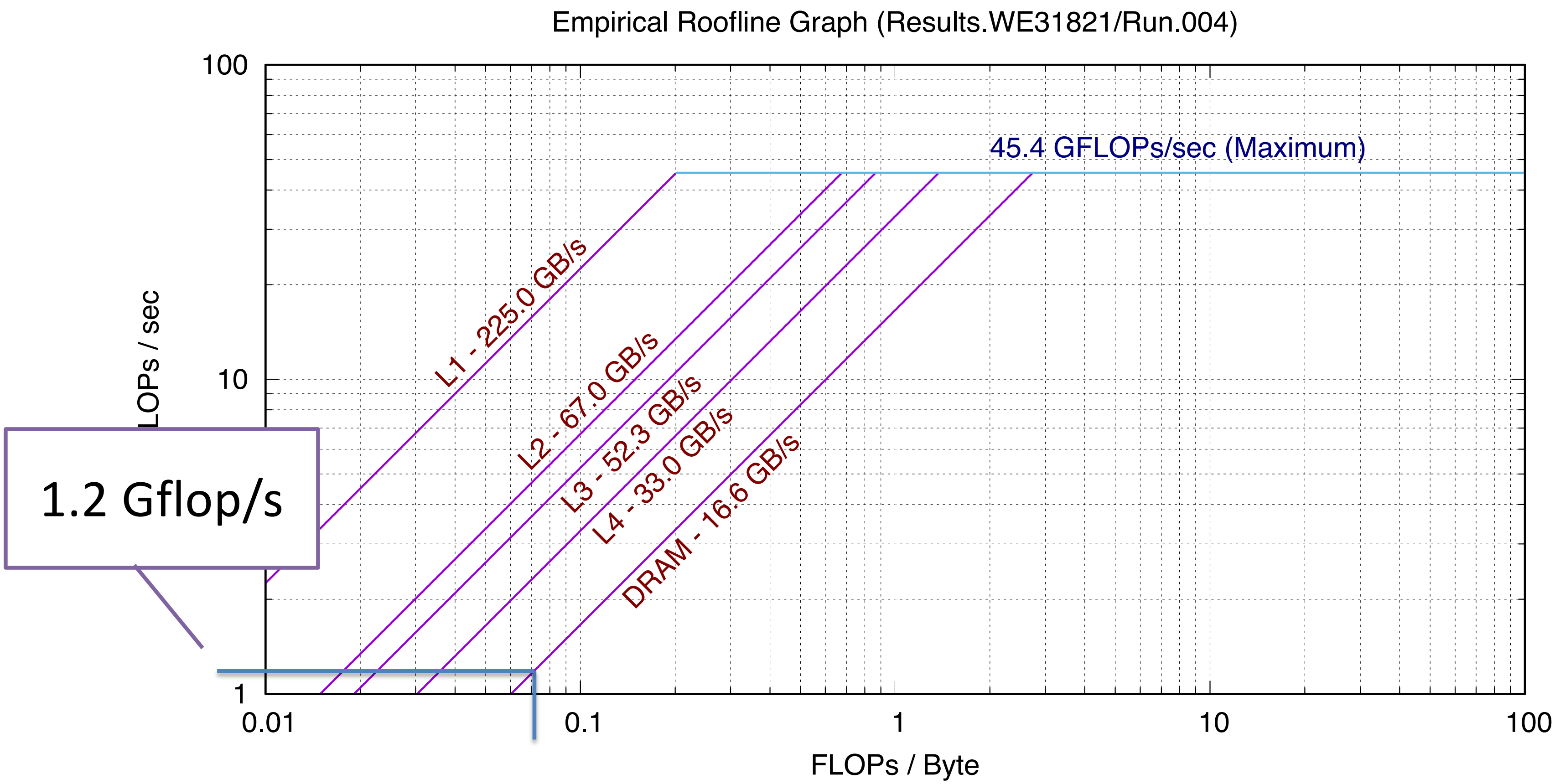
2 NNZ Flops

10N Flops

7N doubles = 56 bytes

10N indexes = 40, 80 bytes

Measured


Empirical Roofline Graph (Results.WE31821/Run.004)
100
10
1
0.01
0.1
1
10
100
FLOPs / Byte
LOPs / sec
45.4 GFLOPs/sec (Maximum)
L1 - 225.0 GB/s
L2 - 67.0 GB/s
L3 - 52.3 GB/s
L4 - 33.0 GB/s
DRAM - 16.6 GB/s
1.2 Gflop/s

Coordinate Storage

```
class COOMatrix {
public:
  COOMatrix(size_t M, size_t N) : num_rows_(M), num_cols_(N) {}

  void matvec(const Vector& x, Vector& y) const {
    for (size_t k = 0; k < storage_.size(); ++k) {
      y(row_indices_[k]) += storage_[k] * x(col_indices[k]);
    }
  }

private:
  int num_rows, num_cols;
  std::vector<size_t> row_indices_, col_indices_;
  std::vector<double> storage_;
};
```

How do we initialize storage_?

In fact, how do we create a sparse matrix?

Filling a Sparse Matrix

```
class COOMatrix {
public:
  COOMatrix(size_t M, size_t N) : num_rows_(M), num_col

  void insert(sizet i, size_t j, double val) {
    row_indices_.push_back(i);
    col_indices_.push_back(j);
    storage_.push_back(val);
  }


private:
  size_t num_rows_, num_cols_;
  std::vector<size_t> row_indices_, col_indices_;
  std::vector<double> storage_;
};
```

Often treated like variable initialization

Matrix is filled with something when created

Can also append elements (no ordering required)

Compressed Sparse Storage

$$\begin{bmatrix} 3 & 0 & 0 & 8 & 0 & 0 \\ 0 & 1 & 4 & 0 & 6 & 0 \\ 0 & 0 & 0 & 0 & 0 & 7 \\ 5 & 0 & 4 & 1 & 0 & 0 \\ 0 & 3 & 0 & 0 & 5 & 0 \\ 0 & 0 & 0 & 0 & 0 & 9 \end{bmatrix}$$

Values repeat

But we can sort the elements by either row index or column index

Each array stores same number of elements (nnz)

row_indices	0	0	1	1	1	2	3	3	3	4	4	5
col_indices	0	3	1	2	4	5	0	2	3	1	4	5
storage	3	8	1	4	6	7	5	4	1	3	5	9

Compressed Sparse Storage

$$\begin{bmatrix} 3 & 0 & 0 & 8 & 0 & 0 \\ 0 & 1 & 4 & 0 & 6 & 0 \\ 0 & 0 & 0 & 0 & 0 & 7 \\ 5 & 0 & 4 & 1 & 0 & 0 \\ 0 & 3 & 0 & 0 & 5 & 0 \\ 0 & 0 & 0 & 0 & 0 & 9 \end{bmatrix}$$

row_indices	4	0	3	0	1	1	3	1	2	3	5	4
col_indices	4	0	2	3	1	2	3	4	5	0	5	1
storage	5	3	4	8	1	4	1	6	7	5	9	3

Unordered elements

row_indices	0	0	1	1	1	2	3	3	3	4	4	5
col_indices	0	3	1	2	4	5	0	2	3	1	4	5
storage	3	8	1	4	6	7	5	4	1	3	5	9

Elements ordered by row

Note all arrays get reordered

Data representing an element stay together

Run Length Encoding of Row Indices

$$\begin{bmatrix} 3 & 0 & 0 & 8 & 0 & 0 \\ 0 & 1 & 4 & 0 & 6 & 0 \\ 0 & 0 & 0 & 0 & 0 & 7 \\ 5 & 0 & 4 & 1 & 0 & 0 \\ 0 & 3 & 0 & 0 & 5 & 0 \\ 0 & 0 & 0 & 0 & 0 & 9 \end{bmatrix}$$

row_indices	0	1	2	3	4	5						
run_length	2	3	1	3	2	1						
col_indices	0	3	1	2	4	5	0	2	3	1	4	5
storage	3	8	1	4	6	7	5	4	1	3	5	9

Do we need this?

Keeps a running total

```
size_t row_ptr = 0;
for (size_t i = 0; i < num_rows_; ++i) {
  for (size_t j = row_ptr; j < row_ptr + row_run_length[i]; ++j)
    y[row_indices_[i]] += storage_[j] * x[col_indices_[j]];
  row_ptr = row_ptr + row_ptr + row_run_length[i];
}
```

Compressed Sparse Row (CSR) Storage

$$\begin{bmatrix} 3 & 0 & 0 & 8 & 0 & 0 \\ 0 & 1 & 4 & 0 & 6 & 0 \\ 0 & 0 & 0 & 0 & 0 & 7 \\ 5 & 0 & 4 & 1 & 0 & 0 \\ 0 & 3 & 0 & 0 & 5 & 0 \\ 0 & 0 & 0 & 0 & 0 & 9 \end{bmatrix}$$

row_indices	0	2	5	6	9	11	12					
col_indices	0	3	1	2	4	5	0	2	3	1	4	5
storage	3	8	1	4	6	7	5	4	1	3	5	9

Store running total instead of computing it

Compressed Sparse Row (CSR) Storage

$$\begin{bmatrix} 3 & 0 & 0 & 8 & 0 & 0 \\ 0 & 1 & 4 & 0 & 6 & 0 \\ 0 & 0 & 0 & 0 & 0 & 7 \\ 5 & 0 & 4 & 1 & 0 & 0 \\ 0 & 3 & 0 & 0 & 5 & 0 \\ 0 & 0 & 0 & 0 & 0 & 9 \end{bmatrix}$$

Size is num_rows_ + 1

One past the end

row_indices	0	2	5	6	9	11	12					
col_indices	0	3	1	2	4	5	0	2	3	1	4	5
storage	3	8	1	4	6	7	5	4	1	3	5	9

row_indices are indices to first element in each row

0	2	5	6	9	11	12

CSR Implementation

Constructor

And row_indices_

Note initial value

Matrix size accessors

Useful info for sparse matrix

Initialize num_rows and num_cols

Private implementation

```
class CSRMatrix {

           ze_t M, size_t N) :  num_rows_(M), num_cols_(N), row_indices_(nu

               ows()     const { return num_rows_; }
               ols()     const { return num_cols_; }
  size_t num_nonzeros() const { return storage_.size(); }

private:
  size_t num_rows_, num_cols_;
  std::vector<size_t> row_indices_, col_indices_;
  std::vector<double> storage_;
};
```

CSR Implementation (Matrix Vector Multiply)

```
class CSRMatrix {

public:
  CSRMatrix(size_t M, size_t N) :  num_rows_(M), num_cols_(N          _rows_+1, 0)  {}

  void matvec(const Vector& x, Vector& y) const {
  for (size_t i = 0; i < num_rows_; ++i) {
    for (size_t j = row_indices_[i]; j < row_indices_[i+1]; ++j) {
      y(i) += storage_[j] * x(col_indices_[j]);
    }
  }
}

private:
  size_t num_rows_, num_cols_;
  std::vector<size_t> row_indices_, col_indices_;
  std::vector<double> storage_;
};
```

For each row

For each element in that row

Row index

Matrix value

Column index

Meditate on this

Building a CSR Matrix

```
class CSRMatrix {

public:
  void open_for_push_back()  { is_open = true; }

  void close_for_push_back() { is_open = false;
    for (size_t i = 0; i < num_rows_; ++i) row_indices_[i+1] += row_indices_[i];
    for (size_t i = num_rows_; i > 0; --i)   row_indices_[i] = row_indices_[i-1];
    row_indices_[0] = 0;
  }

  void push_back(size_t i, size_t j, double value) {
    ++row_indices_[i];
    col_indices_.push_bac
    storage_.push_back(va
  }

private:
  bool is_open;
  size_t num_rows_, num_cols_;
  std::vector<size_t> row_indice
  std::vector<double> storage_;
};
```

When done pushing, accumulate run lengths to offsets

Should be checked

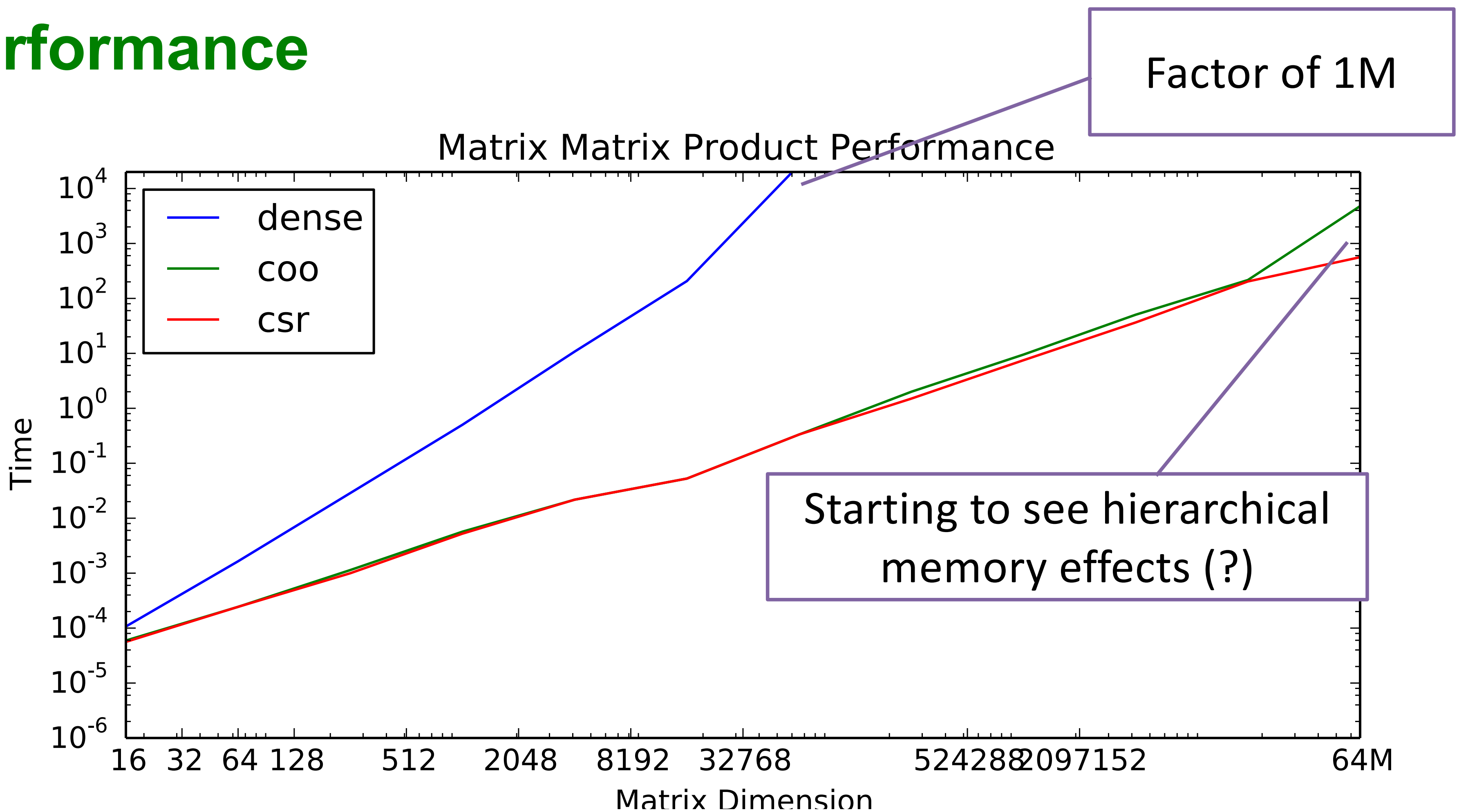
Push elements back (similar to COO)

Accumulate run row lengths

Push column index and value

Rows ***must*** be added in order and contiguously

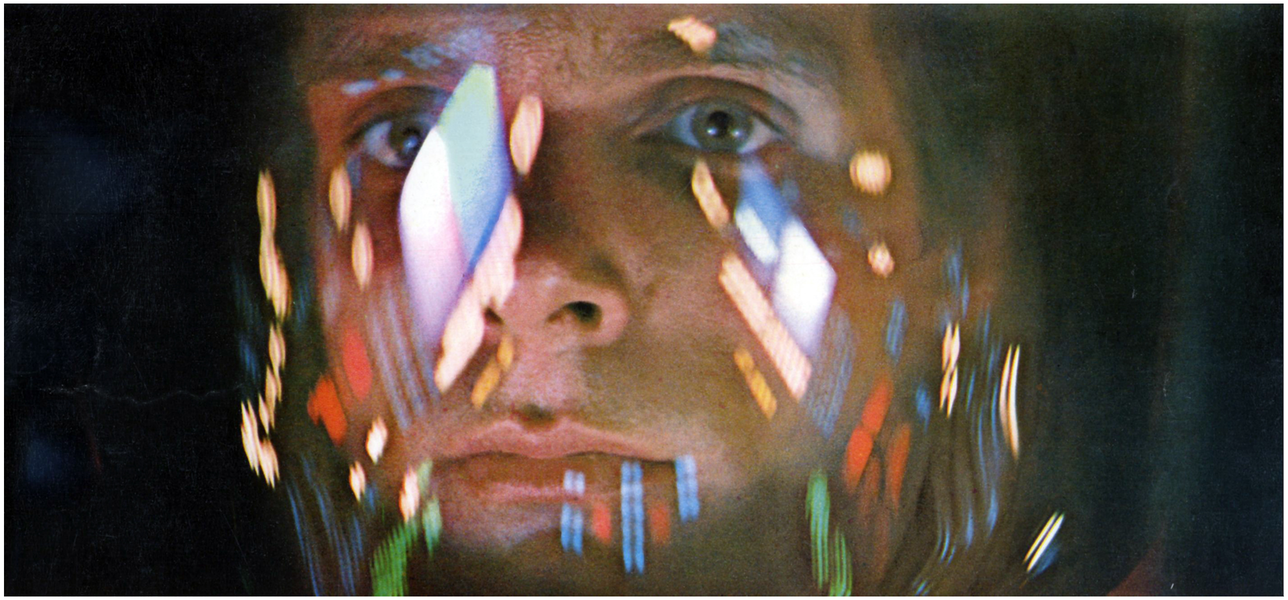
Performance



Review

- Explored variety of techniques for matching algorithm structure to hardware performance features (work smarter)
  - And we pushed this pretty far
- Strassen's algorithm (work way smarter)
- Sparse matrix representations and algorithms (don't do work you don't have to do)
- Get help

Last Chance for Questions Before we Leave the Sequential World



Thank you!

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