CS 470
Spring 2025

Mike Lam, Professor

$$\begin{bmatrix} 1 & 0 & 1 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} ln(l_1) \\ ln(l_2) \\ ln(l_3) \\ ln(l_4) \\ ln(l_5) \\ ln(l_6) \\ ln(l_7) \end{bmatrix} = \begin{bmatrix} ln(r_{1,3,4}) \\ ln(r_{1,3,5}) \\ ln(r_{2,6}) \\ ln(r_{2,7}) \end{bmatrix}$$

Matrices in HPC

(just enough for P2)

Matrices

- Many scientific phenomena can be modeled as matrix operations
  - Differential equations, mesh simulations, view transforms, etc.
  - Many of these phenomena involve solving linear equations
  - Doing this requires linear algebra and the manipulation of large matrices
- Very efficient on vector processors (including GPUs)
  - Data decomposition and SIMD parallelism
  - Small, computation-intensive loop nests called kernels
  - Popular packages: BLAS, LINPACK, LAPACK, ATLAS

$$\begin{bmatrix} 1 & 0 & 1 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} ln(l_1) \\ ln(l_2) \\ ln(l_3) \\ ln(l_4) \\ ln(l_5) \\ ln(l_6) \\ ln(l_7) \end{bmatrix} = \begin{bmatrix} ln(r_{1,3,4}) \\ ln(r_{1,3,5}) \\ ln(r_{2,6}) \\ ln(r_{2,7}) \end{bmatrix}$$

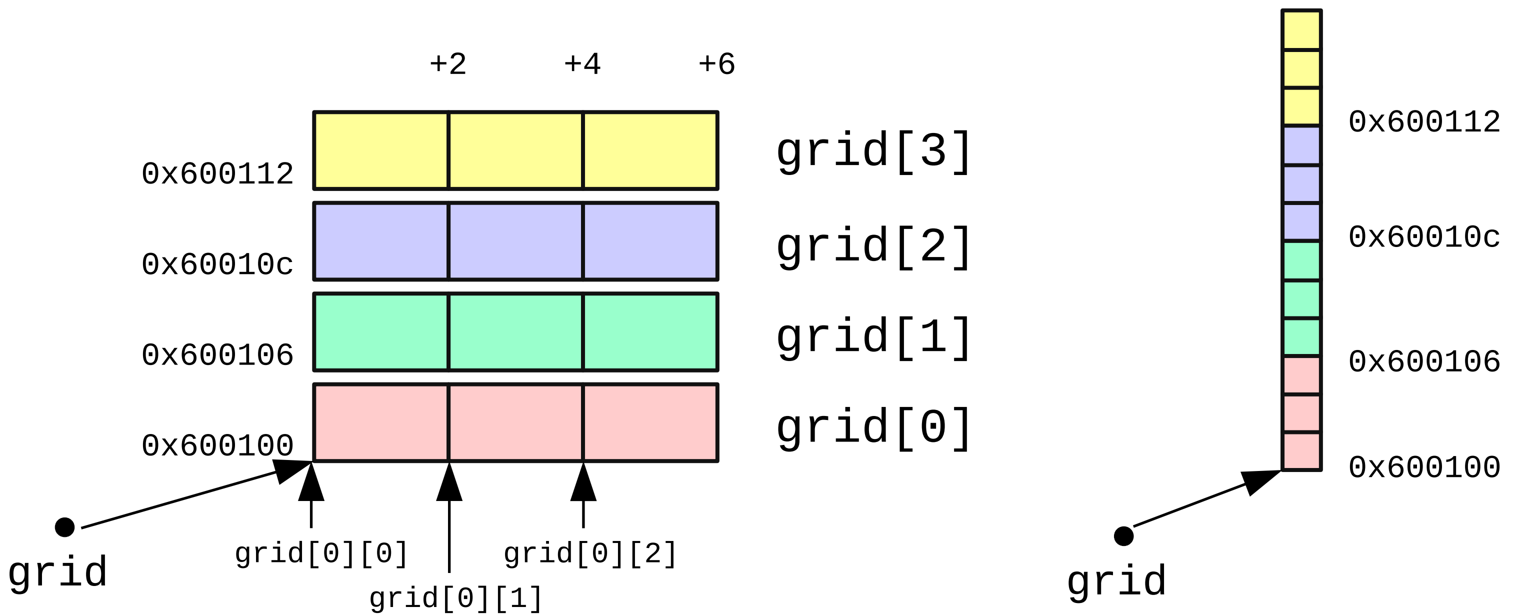
Aside: dense vs. sparse matrices

- A sparse matrix is one in which most elements are zero
  - Could lead to more load imbalances
  - Can be stored more efficiently, allowing for larger matrices
  - Dense/normal matrix operations no longer work
  - It is a challenge to make sparse operations as efficient as dense operations

$$\begin{pmatrix} 11 & 22 & 0 & 0 & 0 & 0 & 0 \\ 0 & 33 & 44 & 0 & 0 & 0 & 0 \\ 0 & 0 & 55 & 66 & 77 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 88 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 99 \end{pmatrix}$$

Matrix representation

- 2D dense row-major matrices in C/C++
  - Often stored in 1D arrays w/ access via array index arithmetic
  - "Row-major" order: outer dimension specified first
  - Address of (*i*,*j*)th element is $(\text{base} + \text{size}(i * \text{cols} + j))$



Matrix representation

- Parallelism w/ 2D matrices
  - Your goals: 1) **analyze**, 2) **parallelize** (w/ OpenMP), and 3) **evaluate**
  - Example (matrix multiplication):

```
void multiply_matrices(int *A, int *B, int *R, int n)
{
    int i, j, k;
    for (i = 0; i < n; i++) {
        for (j = 0; j < n; j++) {
            R[i*n+j] = 0;
            for (k = 0; k < n; k++) {
                R[i*n+j] += A[i*n+k] * B[k*n+j];
            }
        }
    }
}
```

Matrix representation

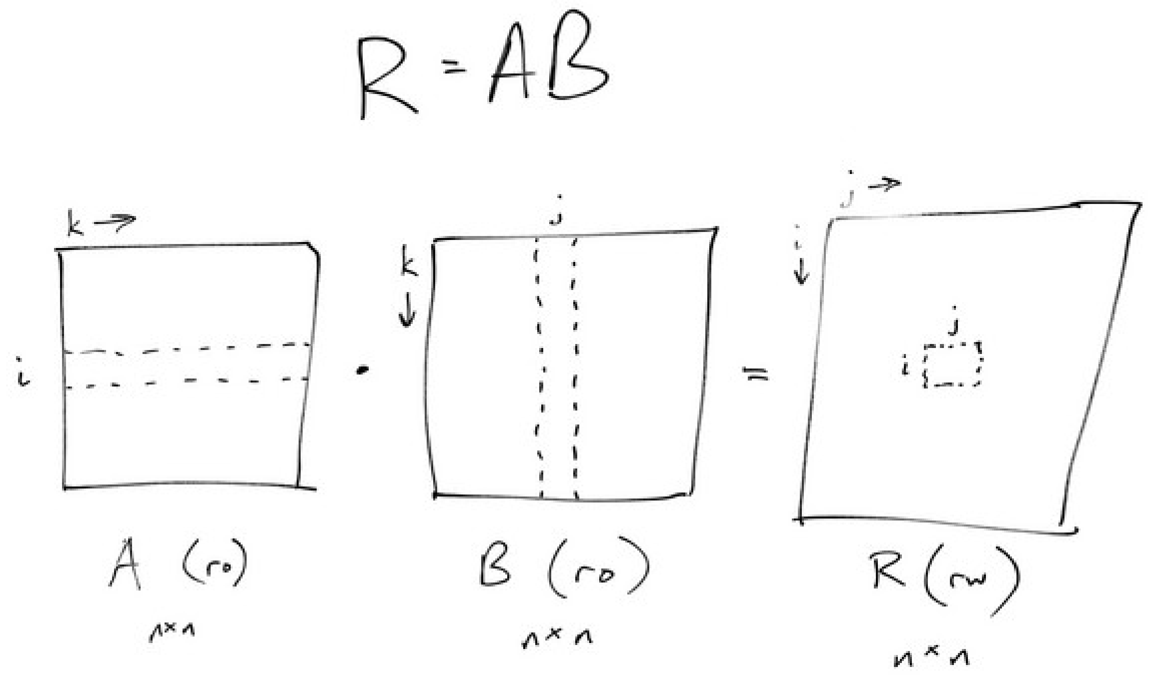
- Parallelism w/ 2D matrices
  - Your goals: 1) **analyze**, 2) **parallelize** (w/ OpenMP), and 3) **evaluate**
  - Example (matrix multiplication):

```
void multiply_matrices(int *A, int *B, int *R, int n)
{
    int i, j, k;
    for (i = 0; i < n; i++) {
        for (j = 0; j < n; j++) {
            R[i*n+j] = 0;
            for (k = 0; k < n; k++) {
                R[i*n+j] += A[i*n+k] * B[k*n+j];
            }
        }
    }
}
```

read as `R[i][j]`

Matrix access patterns

```
void multiply_matrices(int *A, int *B, int *R, int n)
{
    int i, j, k;
    for (i = 0; i < n; i++) {
        for (j = 0; j < n; j++) {
            R[i*n+j] = 0;
            for (k = 0; k < n; k++) {
                R[i*n+j] += A[i*n+k] * B[k*n+j];
            }
        }
    }
}
```



Matrix access patterns

```
void multiply_matrices(int *A, int *B, int *R, int n)
{
    int i, j, k;
    for (i = 0; i < n; i++) {
        for (j = 0; j < n; j++) {
            R[i*n+j] = 0;
#           pragma omp parallel for default(none) \
                shared(A,B,R,n,i,j) private(k)
            for (k = 0; k < n; k++) {
                R[i*n+j] += A[i*n+k] * B[k*n+j];
            }
        }
    }
}
```

Incorrect b/c of loop-carried dependencies

```
== SERIAL ==
Nthreads= 1  TEST=pass  MULT=  0.7825
== PARALLEL ==
Nthreads= 1  TEST=pass  MULT=  1.0443
Nthreads= 2  TEST=FAIL  MULT=  2.3410
Nthreads= 4  TEST=FAIL  MULT=  3.7809
Nthreads= 8  TEST=FAIL  MULT=  6.5935
Nthreads=16  TEST=FAIL  MULT=  9.2631
Nthreads=32  TEST=FAIL  MULT= 17.3672
```

Matrix access patterns

```
void multiply_matrices(int *A, int *B, int *R, int n)
{
    int i, j, k;
    for (i = 0; i < n; i++) {
        for (j = 0; j < n; j++) {
            int tmp = 0;
#           pragma omp parallel for default(none) \
                reduction(+:tmp) shared(A,B,R,n,i,j) private(k)
            for (k = 0; k < n; k++) {
                tmp += A[i*n+k] * B[k*n+j];
            }
            R[i*n+j] = tmp;
        }
    }
}
```

Correct w/ no speedup

```
== SERIAL ==
Nthreads= 1  TEST=pass  MULT=  0.7308
== PARALLEL ==
Nthreads= 1  TEST=pass  MULT=  1.0136
Nthreads= 2  TEST=pass  MULT=  2.2375
Nthreads= 4  TEST=pass  MULT=  4.1329
Nthreads= 8  TEST=pass  MULT=  7.6924
Nthreads=16  TEST=pass  MULT=  8.8584
Nthreads=32  TEST=pass  MULT= 16.4827
```

Matrix access patterns

```
void multiply_matrices(int *A, int *B, int *R, int n)
{
    int i, j, k;
    for (i = 0; i < n; i++) {
#       pragma omp parallel for default(none) shared(A,B,R,n,i) private(j,k)
        for (j = 0; j < n; j++) {
            R[i*n+j] = 0;
            for (k = 0; k < n; k++) {
                R[i*n+j] += A[i*n+k] * B[k*n+j];
            }
        }
    }
}
```

Correct w/ speedup

```
== SERIAL ==
Nthreads= 1  TEST=pass  MULT=  0.7669
== PARALLEL ==
Nthreads= 1  TEST=pass  MULT=  0.7816
Nthreads= 2  TEST=pass  MULT=  0.3983
Nthreads= 4  TEST=pass  MULT=  0.1991
Nthreads= 8  TEST=pass  MULT=  0.1032
Nthreads=16  TEST=pass  MULT=  0.1060
Nthreads=32  TEST=pass  MULT=  0.0785
```

Matrix access patterns

```
void multiply_matrices(int *A, int *B, int *R, int n)
{
    int i, j, k;
#   pragma omp parallel for default(none) shared(A,B,R,n) private(i,j,k)
    for (i = 0; i < n; i++) {
        for (j = 0; j < n; j++) {
            R[i*n+j] = 0;
            for (k = 0; k < n; k++) {
                R[i*n+j] += A[i*n+k] * B[k*n+j];
            }
        }
    }
}
```

Correct w/ best speedup
(fewest fork/join operations)

```
== SERIAL ==
Nthreads= 1  TEST=pass  MULT=  0.7861
== PARALLEL ==
Nthreads= 1  TEST=pass  MULT=  0.7921
Nthreads= 2  TEST=pass  MULT=  0.3978
Nthreads= 4  TEST=pass  MULT=  0.1957
Nthreads= 8  TEST=pass  MULT=  0.1043
Nthreads=16  TEST=pass  MULT=  0.0908
Nthreads=32  TEST=pass  MULT=  0.0640
```

HPL benchmark

- HPL: LINPACK-based dense linear algebra benchmark
  - Generation of a linear system of equations "Ax = b" - $O(n^2)$
    - Choose 'b' such that 'x' (answer vector) values are known
    - Distribute dense matrix 'A' in block-cyclic pattern
  - LU factorization - $O(n^3)$
  - Backward substitution to solve system - $O(n^2)$
  - Error calculation to verify correctness - $O(n)$
  - Calculate max sustained FLOPS (*floating-point operations per second*)
    - Usually significantly less than theoretical machine peak (Rmax vs Rpeak)
    - Serves as proxy app for target workloads (similar characteristics)
    - Used to rank world's fastest systems on the Top500 list twice each year
  - ~~Compiled on cluster~~
    - ~~Located in `/shared/apps/hpl-2.1/bin/Linux_PII_CBLAS`~~

P2 (OpenMP)

- Similar to HPL benchmark
  1) Random generation of linear system (x should be all 1's)
  2) Gaussian elimination (similar to LU factorization)
  3) Backwards substitution (row- or column-oriented)

Non-random example

$$\begin{aligned} 3x + 2y - z &= 1 \\ 2x - 2y + 4z &= -2 \\ -x + \tfrac{1}{2}y - z &= 0 \end{aligned}$$

Original system (Ax = b)

$$\left[\begin{array}{rrr|r} 3.0 & 2.0 & -1.0 & 1.0 \\ 2.0 & -2.0 & 4.0 & -2.0 \\ -1.0 & 0.5 & -1.0 & 0.0 \end{array}\right]$$

Augmented matrix [A | b]

Gaussian elimination

$$\left[\begin{array}{rrr|r} 3.0 & 2.0 & -1.0 & 1.0 \\ 0.0 & -3.3 & 4.7 & -2.7 \\ 0.0 & 0.0 & 0.3 & -0.6 \end{array}\right]$$

Upper triangular system

Backward substitution

$$\left[\begin{array}{rrr|r} 1.0 & 0.0 & 0.0 & 1.0 \\ 0.0 & 1.0 & 0.0 & -2.0 \\ 0.0 & 0.0 & 1.0 & -2.0 \end{array}\right]$$

Solved system