An Introduction to Parallel Computing:
Portable Shared Memory Parallel Programming with OpenMP

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Student Cluster Competition Training Session
Friday, April 26th, 2019
1:00PM - 3:00PM PT

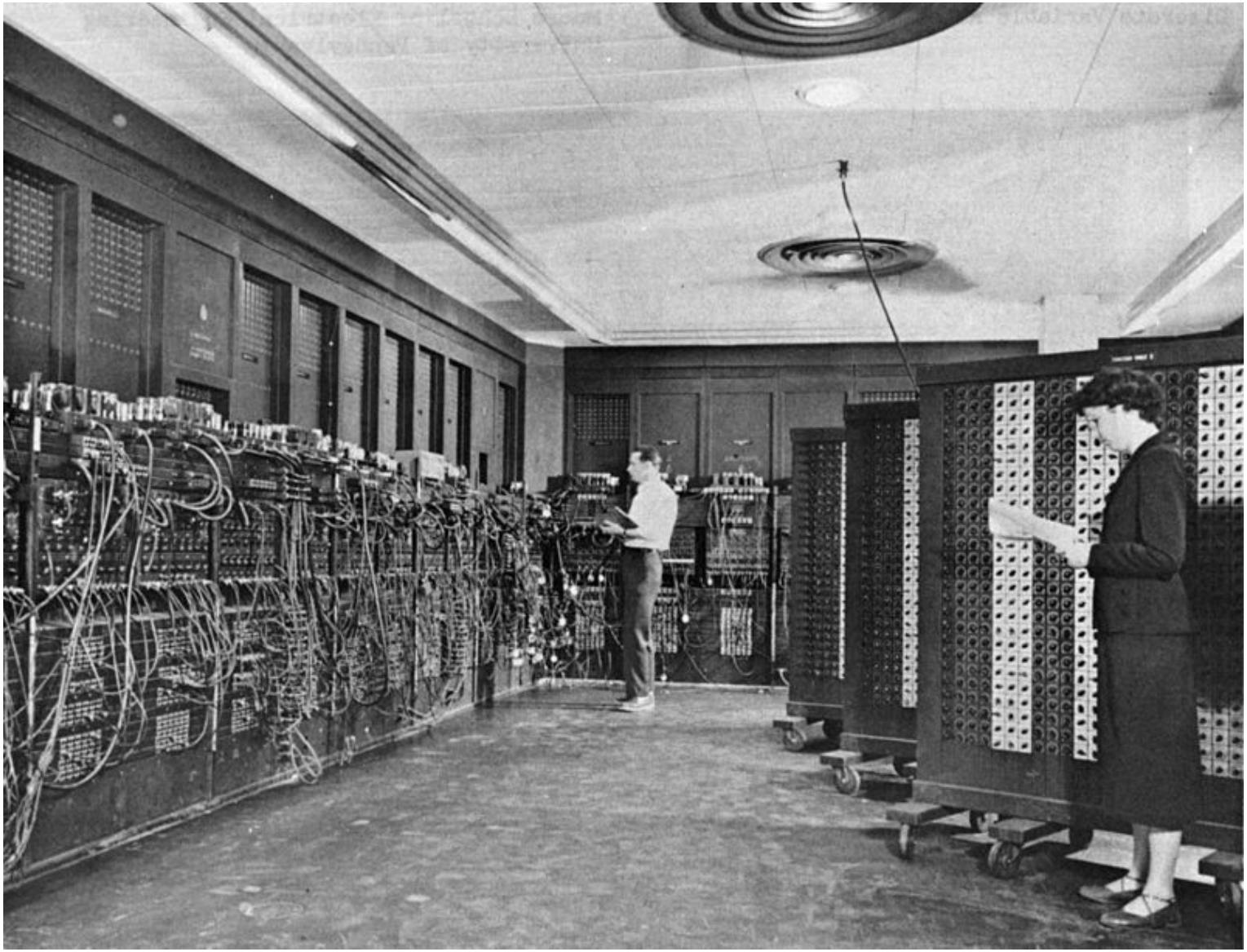
About Me

- B.S. in Physics + Applied Mathematics (Michigan); undergraduate research: experimental physics
- M.S. in Physics, Ph.D. Computational Science (SDSU); graduate research: computational/theoretical physics
- Started working in Data Center Operations Group @ SDSC while finishing Ph.D.
- Previously worked for Distributed High-Throughput Computing Group @ SDSC and the Open Science Grid
- Joined HPC User Services Group @ SDSC in April 2017

An Overview of Today's Training Session

- A Brief History of Computation
- Serial Computation and its Limits
- Parallel Computation and its Limits
- An Introduction to OpenMP
- Advanced Code Optimization with OpenMP
- Q&A?

A Brief History of Computation

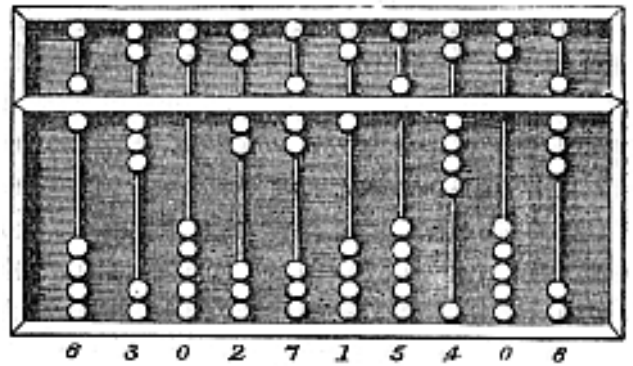


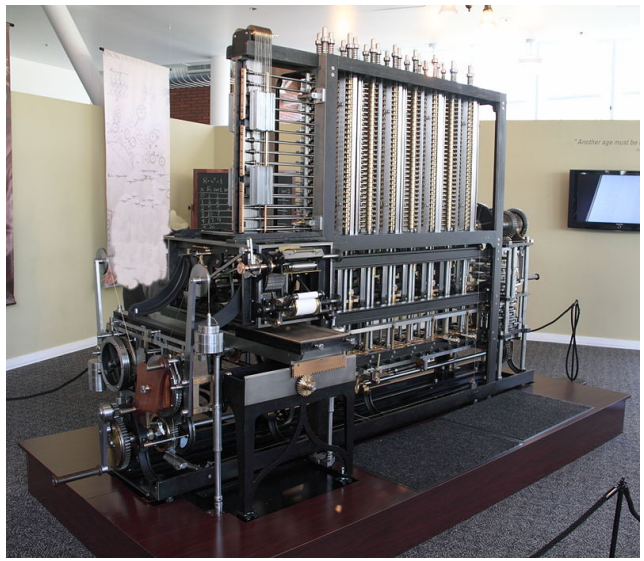
What is a Computer?

- A **computer** is a machine that can be instructed to carry out a sequence of operations – often arithmetic or logic operations — to accomplish a specific task or set of tasks.
- A computer **program** is the set of instructions or operations that perform a specific task or set of tasks executed by a computer.

The Mechanical Age of Computing

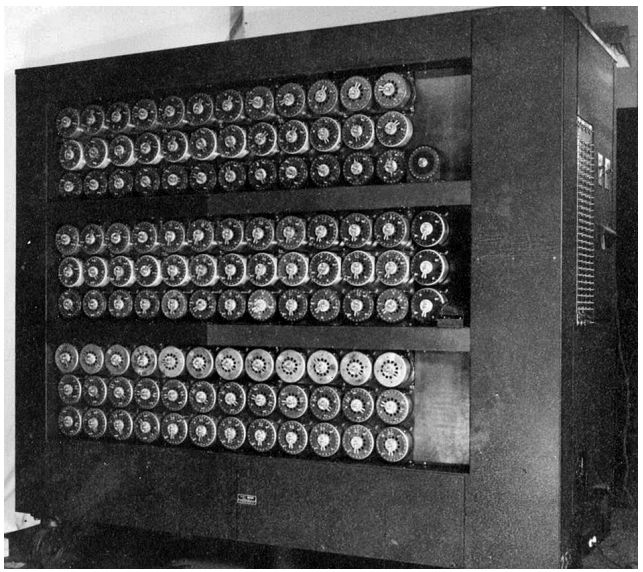
- 2700-2300 BCE: Earliest known use of the abacus
- 1050-771 BCE: Earliest known use of an analog computer
- 1642: First mechanical calculator
- 1725: First punch card system
- 1837: First design for a general-purpose computer
- 1843: First design of a computer program





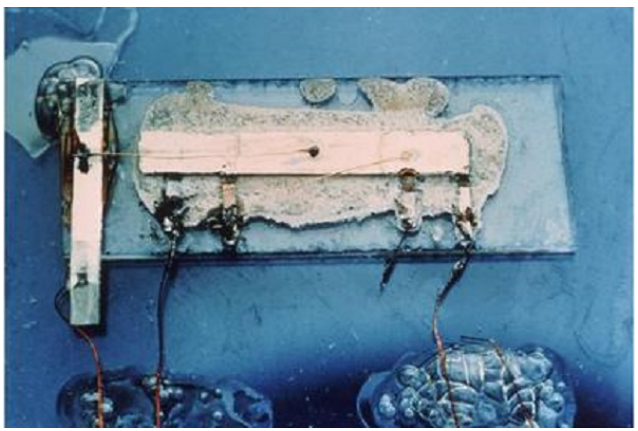
The Electro-Mechanical Age of Computing

- 1890: First use of a punch card system to compute the U.S. Census
- 1911: Founding of International Business Machines Corporation
- 1939: First Polish bombe begins deciphering German Enigma messages



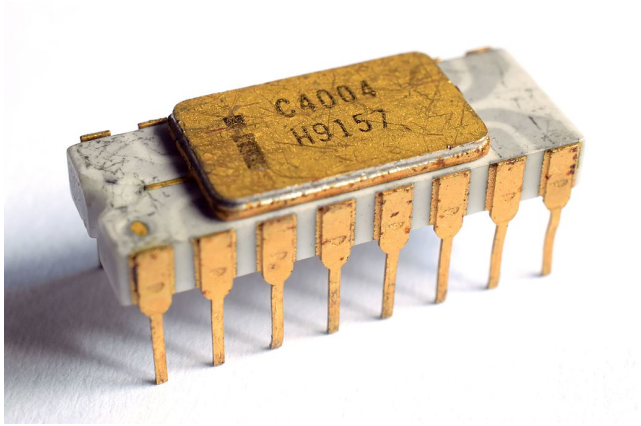
The Electronic Age of Computing

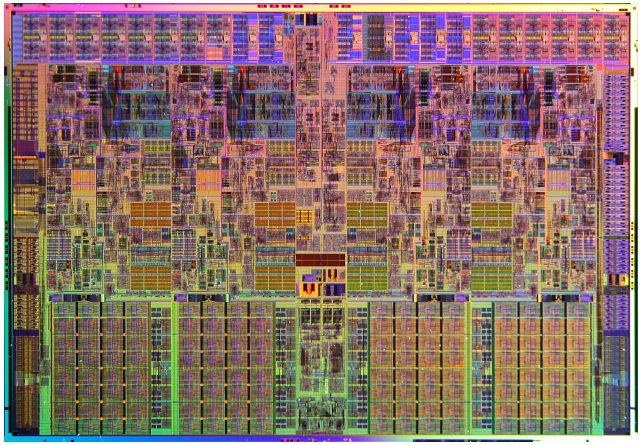
- 1936: First description of a universal Turing machine
- 1945: First electronic, general-purpose computer; von Neumann computer architecture
- 1947: First transistor
- 1951: First parallel computer
- 1953: First high-level computer programming language
- 1958: First integrated circuit; First computer network



The Electronic Age of Computing

- 1961: First all-transistor supercomputer
- 1965: First description of Moore's Law
- 1969: First link of ARPANET established
- 1971: First microprocessor
- 1973: First public release of the Unix operating system
- 1989: First public Internet service provider





Serial Computation and its Limits

Parallel Computation and its Limits

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https://computing.llnl.gov/tutorials/parallel_comp/

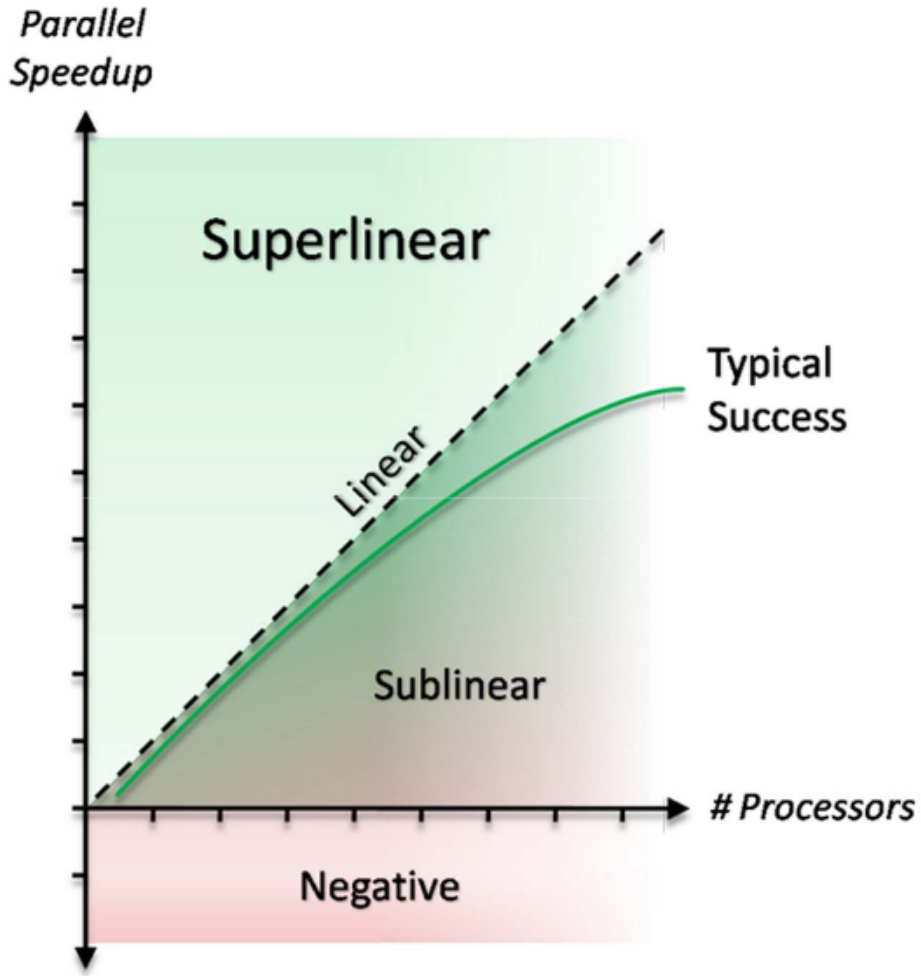
Parallel Speedup

- Parallel speedup measures how much faster a parallel algorithm solves a given problem compared to its sequential version.
- Parallel speedup is defined as

$$S_n = \frac{T_1}{T_n},$$

where T_1 is the execution runtime of the sequential algorithm on a single processing unit and T_n is the execution runtime of the parallel algorithm on n processing units.

- In general, we expect $T_1 > T_n$ such that $S_n > 1$.



Parallel Efficiency

- Parallel efficiency measures how well-utilized the hardware processing units are in solving a given problem.
- Parallel efficiency is defined as

$$E_n = \frac{S_n}{n} = \frac{T_1}{nT_n}.$$

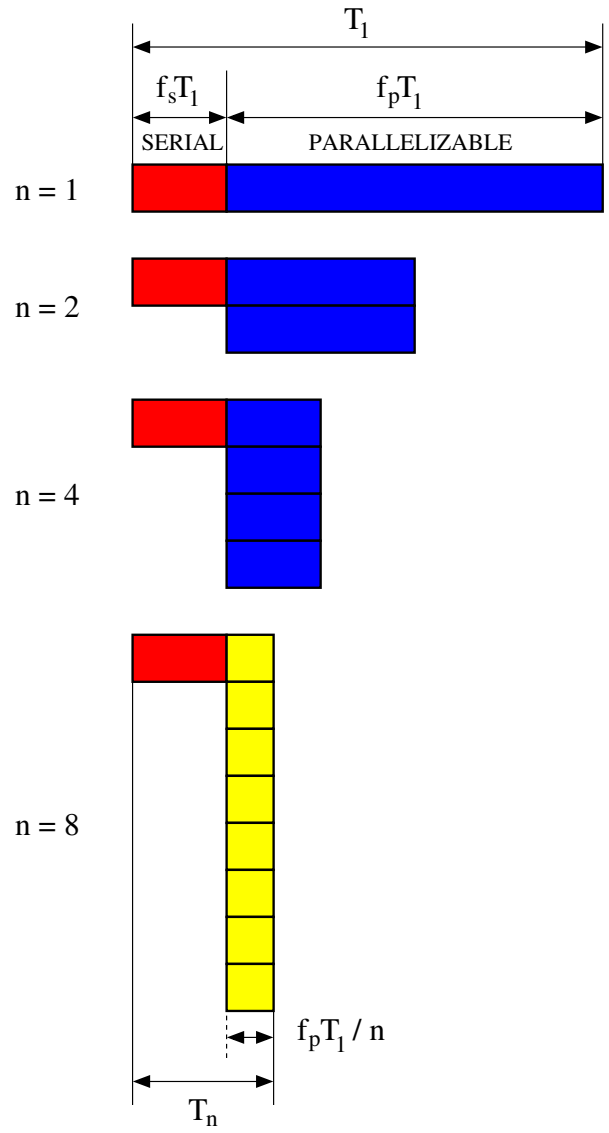
- Therefore, $0 \leq E_n \leq 1$ measures the fraction of time a processing unit performs useful work.

Strong Scalability and Amdahl's Law

- Strong scalability measures how the time-to-solution for a problem varies as a function of the number of processing units when the *problem size is fixed*.
- Strong scalability is limited by Amdahl's law, which states that the theoretical speedup of a parallel algorithm is given by

$$S_n = \frac{1}{f_s + \frac{f_p}{n}},$$

where f_p is the fraction of an algorithm's instructions that can be executed in parallel, while f_s is the fraction of instructions that must be executed sequentially.



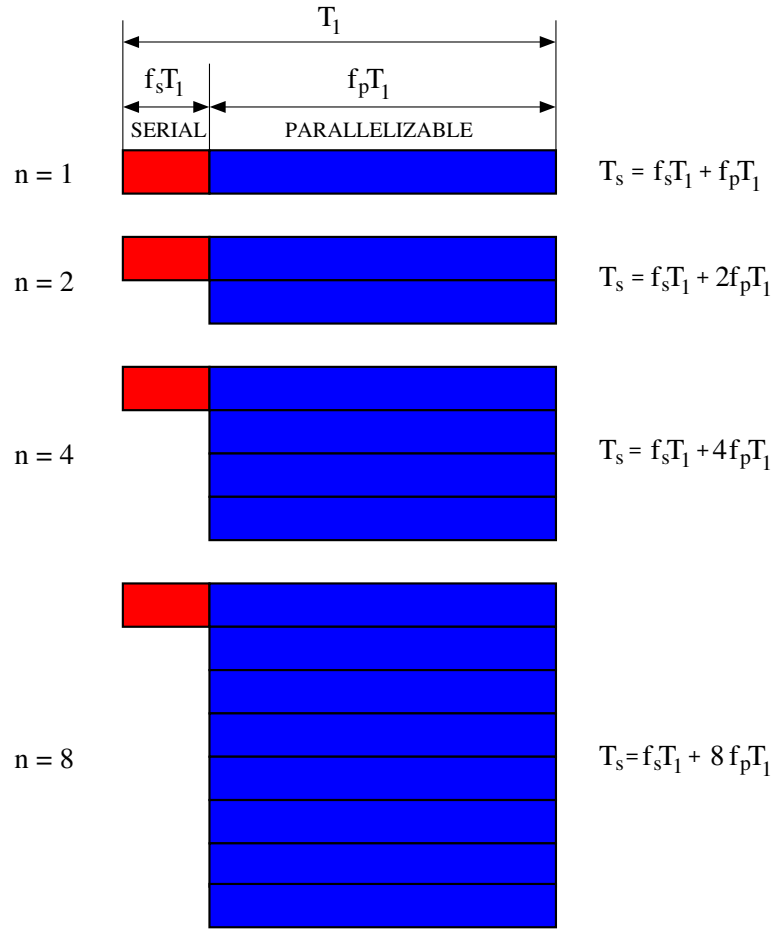
Weak Scalability and Gustafson's Law

- Weak scalability measures how the time-to-solution for a problem varies as a function of the number of processing units when there is a *fixed problem size per processing unit*.
- Weak scalability is limited by Gustafson's Law, which states that the theoretical speedup of a parallel algorithm is given by

$$S_n = n - f_s^*(n-1),$$

where $0 \leq f_s^* \leq 1$ is the sequential fraction of the parallel execution runtime. Note: $f_s^* \neq f_s$.

- If $f_s^* \to 0$, then $S_n \to n$.



An Introduction to OpenMP

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https://computing.llnl.gov/tutorials/openMP

hello, world (c)

```c
#include <stdio.h>

int main(void) {

    printf("hello, world\n");
    return 0;

}
```

hello, shared memory world (c)

```c
#include <stdio.h>
#include <omp.h>

int main(void) {

    int number_of_threads, thread_id;

    #pragma omp parallel private(thread_id)
    {
        thread_id = omp_get_thread_num();

        #pragma omp master
        {
            number_of_threads = omp_get_num_threads();
        }

        #pragma omp barrier
        printf("hello, shared memory world from thread %d of \
            %d\n", thread_id, number_of_threads);
    }

    return 0;

}
```

hello, world (fortran)

```
program hello

use, intrinsic :: iso_fortran_env
implicit none

write(unit=output_unit, fmt=*) "hello, world"

stop

end program hello
```

hello, shared memory world (fortran)

```
      program hello_omp

      use, intrinsic :: iso_fortran_env
      implicit none

      integer :: number_of_threads, thread_id
      integer :: omp_get_num_threads, omp_get_thread_num

!$omp parallel private(thread_id)
      thread_id = omp_get_thread_num()
!$omp master
      number_of_threads = omp_get_num_threads()
!$omp end master
!$omp barrier
      write(unit=output_unit, fmt=*) "hello, shared memory&
         & world from thread ", thread_id, " of ",&
         & number_of_threads
!$omp end parallel

      stop

      end program hello_omp
```

Matrix-Vector Multiplication

$$\mathbf{y} = \mathbf{A}\mathbf{x}$$

Matrix-Vector Multiplication

$$\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$$

Matrix-Vector Multiplication

$$\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{bmatrix} = \begin{bmatrix} a_{11}x_1 + a_{12}x_2 + \cdots + a_{1n}x_n \\ a_{21}x_2 + a_{22}x_2 + \cdots + a_{2n}x_n \\ \vdots \\ a_{m1}x_1 + a_{m2}x_2 + \cdots + a_{mn}x_n \end{bmatrix}$$

Matrix-Vector Multiplication

$$y_i = \sum_{j=1}^{n} a_{ij} x_j$$

where $i = 1, 2, \ldots, m$.

Hilbert Matrix

A Hilbert matrix is a square matrix with elements that are unit fractions given by

$$H_{ij} = \frac{1}{i + j - 1}$$

For example, the Hilbert matrix of dimension 4 is

$$\mathbf{H} = \begin{bmatrix} 1 & 1/2 & 1/3 & 1/4 \\ 1/2 & 1/3 & 1/4 & 1/5 \\ 1/3 & 1/4 & 1/5 & 1/6 \\ 1/4 & 1/5 & 1/6 & 1/7 \end{bmatrix}$$

Exercise: Matrix-Vector Multiplication

If $\mathbf{H}$ is a Hilbert matrix of dimension $n = 122880$ and $\mathbf{x} = [1 \cdots 1]^T$ is an all-ones vector of the same dimension, compute the resultant vector $\mathbf{y} = \mathbf{H}\mathbf{x}$.

Check your result by computing the sum of the elements of $\mathbf{y}$. For $\mathbf{H}$ and $\mathbf{x}$ of dimension n, the sum of the elements of $\mathbf{y}$ is given analytically by

$$\sum_{i=1}^{n} y_i = n + \sum_{j=1}^{n-1} \frac{n-j}{n+j}.$$

Extra credit: Optimize your code and recompute for both $n = 122880$ and $n = 1048576$. Plot the parallel speedup and efficiency of your code.

Questions?