# CS 470
# Spring 2016

Mike Lam, Professor


# Other Architectures

*(with an aside on linear algebra)*

# Parallel Systems

- Shared memory (uniform global address space)
  - Primary story: make faster computers
  - Programming paradigm: threads
  - Technologies: Pthreads, OpenMP
- Distributed (Non-Uniform Memory Access – *NUMA*)
  - Primary story: add more computers
  - Programming paradigm: message passing
  - Technologies: MPI (OpenMPI/MPICH), SLURM

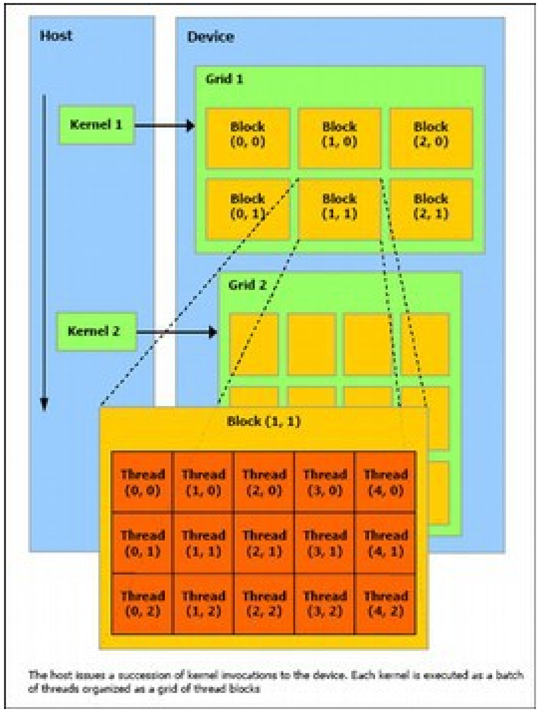
*Where do we go from here?*

# A brief digression into gaming

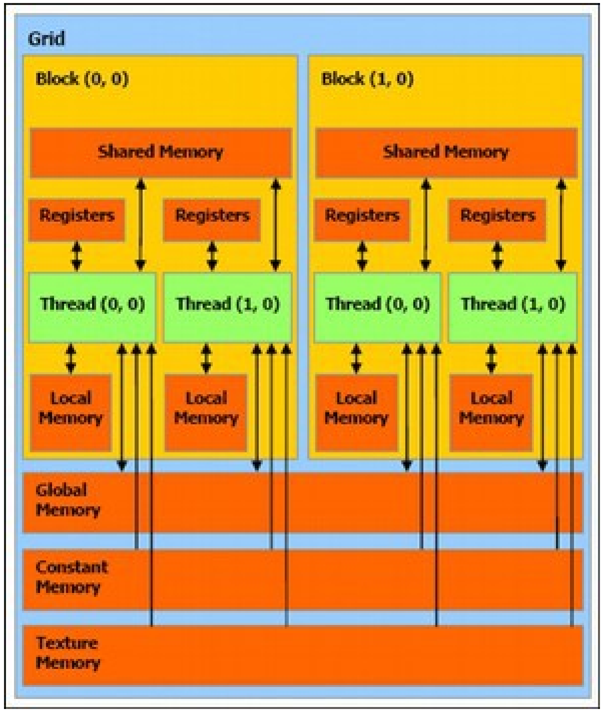
- **1970s**: arcades began using specialized graphics chips
- **1980s**: increasingly sophisticated capabilities (e.g., sprites, blitters, scrolling)
- Early-mid **1990s**: first 3D consoles (e.g., N64) and 3D accelerator cards for PCs
- Late **1990s**: classic wars begin: Nvidia vs. ATI and DirectX vs. OpenGL
- Early **2000s**: creation of "shaders" (easier non-graphical use of accelerators)
- Late **2000s**: rise of General-Purpose GPU (GPGPU) frameworks
  - 2007: Compute Unified Device Architecture (CUDA) released (newer library: Thrust)
  - 2009: OpenCL standard released
  - 2011: OpenACC standard released

# GPU Programming

- "*Kernels*" run on a batch of threads
  - Distributed onto many low-powered GPU cores
  - Grouped into *blocks* of cores and *grids* of blocks
  - Limited instruction set that operates on vector data
  - Must copy data to/from main memory




The host issues a succession of kernel invocations to the device. Each kernel is executed as a batch of threads organized as a grid of thread blocks



# GPU Programming (CUDA)

```
void saxpy_serial(int n, float a, float *x, float *y)
{
    for (int i = 0; i < n; ++i)
        y[i] = a*x[i] + y[i];
}

// Invoke serial SAXPY kernel
saxpy_serial(n, 2.0, x, y);
```

Low-level control of parallelism on GPU

```
__global__ void saxpy_parallel(int n, float a, float *x, float *y)
{
    int i = blockIdx.x*blockDim.x + threadIdx.x;
    if (i < n) y[i] = a*x[i] + y[i];
}

// Invoke parallel SAXPY kernel with 256 threads/block
int nblocks = (n + 255) / 256;
saxpy_parallel<<<nblocks, 256>>>(n, 2.0, x, y);
```

# GPU Programming (CUDA)

```
// Kernel that executes on the CUDA device
__global__ void square_array(float *a, int N)
{
  int idx = blockIdx.x * blockDim.x + threadIdx.x;
  if (idx<N) a[idx] = a[idx] * a[idx];
}

// main routine that executes on the host
int main(void)
{
  float *a_h, *a_d;  // Pointer to host & device arrays
  const int N = 10;  // Number of elements in arrays
  size_t size = N * sizeof(float);
  a_h = (float *)malloc(size);        // Allocate array on host
  cudaMalloc((void **) &a_d, size);   // Allocate array on device

  // Initialize host array and copy it to CUDA device
  for (int i=0; i<N; i++) a_h[i] = (float)i;
  cudaMemcpy(a_d, a_h, size, cudaMemcpyHostToDevice);

  // Do calculation on device:
  int block_size = 4;
  int n_blocks = N/block_size + (N%block_size == 0 ? 0:1);
  square_array <<< n_blocks, block_size >>> (a_d, N);

  // Retrieve result from device and store it in host array
  cudaMemcpy(a_h, a_d, sizeof(float)*N, cudaMemcpyDeviceToHost);

  // Print results and cleanup
  for (int i=0; i<N; i++) printf("%d %f\n", i, a_h[i]);
  free(a_h); cudaFree(a_d);
}
```

Must micromanage memory usage and data movement

NVIDIA CUDA

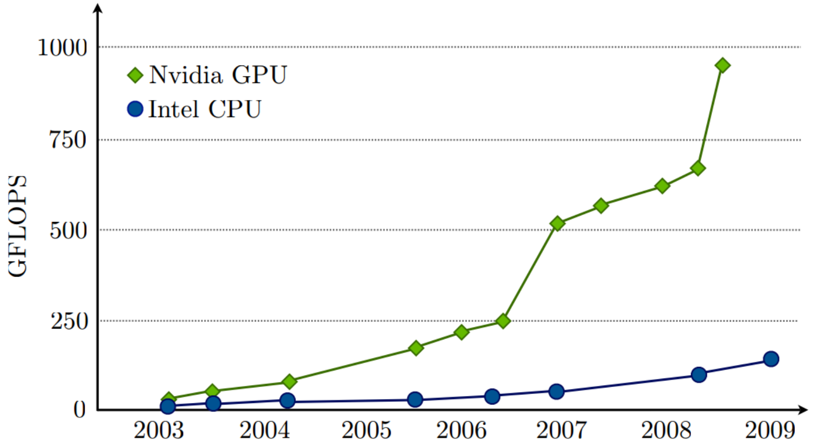
# GPU Programming (OpenACC)

```
#pragma acc data copy(A) create(Anew)
while (error > tol && iter < iter_max)  {
  error = 0.0;

  #pragma acc kernels
  {
    #pragma acc loop
    for (int j = 1; j < n-1; j++) {
      for (int i = 1; i < m-1; i++) {
         Anew[j][i] = 0.25 * (A[j][i+1] + A[j][i-1] +
                              A[j-1][i] + A[j+1][i];
         error = fmax(error, fabs(Anew[j][i] - A[j][i]));
      }
    }

    #pragma acc loop
    for (int j = 1; j < n-1; j++) {
      for (int = i; i < m-1; i++ ) {
        A[j][i] = Anew[j][i];
      }
    }
  }

  if (iter % 100 == 0) printf("%5d, %0.6f\n", iter, error);
  iter++;
}
```

Fewer modifications required; may not parallelize effectively

# Hybrid HPC architectures

- Highly parallel on the node
  - Hardware: CPU w/ accelerators
    - GPUs or manycore processors (e.g., Intel Phi and SunWay)
  - Technologies: OpenMP, CUDA, OpenACC, OpenCL
- Distributed between nodes
  - Hardware: interconnect and distributed FS
  - Technologies: Infiniband, Lustre, HDFS



# Top10 systems (Spring 2016)

| RANK | SITE | SYSTEM | CORES | RMAX (TFLOP/S) | RPEAK (TFLOP/S) | POWER (KW) |
|---|---|---|---|---|---|---|
| 1 | National Super Computer Center in Guangzhou<br>China | **Tianhe-2 (MilkyWay-2)** - TH-IVB-FEP Cluster, Intel Xeon E5-2692 12C 2.200GHz, TH Express-2, Intel Xeon Phi 31S1P<br>NUDT | 3,120,000 | 33,862.7 | 54,902.4 | 17,808 |
| 2 | DOE/SC/Oak Ridge National Laboratory<br>United States | **Titan** - Cray XK7 , Opteron 6274 16C 2.200GHz, Cray Gemini interconnect, NVIDIA K20x<br>Cray Inc. | 560,640 | 17,590.0 | 27,112.5 | 8,209 |
| 3 | DOE/NNSA/LLNL<br>United States | **Sequoia** - BlueGene/Q, Power BQC 16C 1.60 GHz, Custom<br>IBM | 1,572,864 | 17,173.2 | 20,132.7 | 7,890 |
| 4 | RIKEN Advanced Institute for Computational Science (AICS)<br>Japan | K computer, SPARC64 VIIIfx 2.0GHz, Tofu interconnect<br>Fujitsu | 705,024 | 10,510.0 | 11,280.4 | 12,660 |
| 5 | DOE/SC/Argonne National Laboratory<br>United States | **Mira** - BlueGene/Q, Power BQC 16C 1.60GHz, Custom<br>IBM | 786,432 | 8,586.6 | 10,066.3 | 3,945 |
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| 10 | Texas Advanced Computing Center/Univ. of Texas<br>United States | **Stampede** - PowerEdge C8220, Xeon E5-2680 8C 2.700GHz, Infiniband FDR, Intel Xeon Phi SE10P<br>Dell | 462,462 | 5,168.1 | 8,520.1 | 4,510 |

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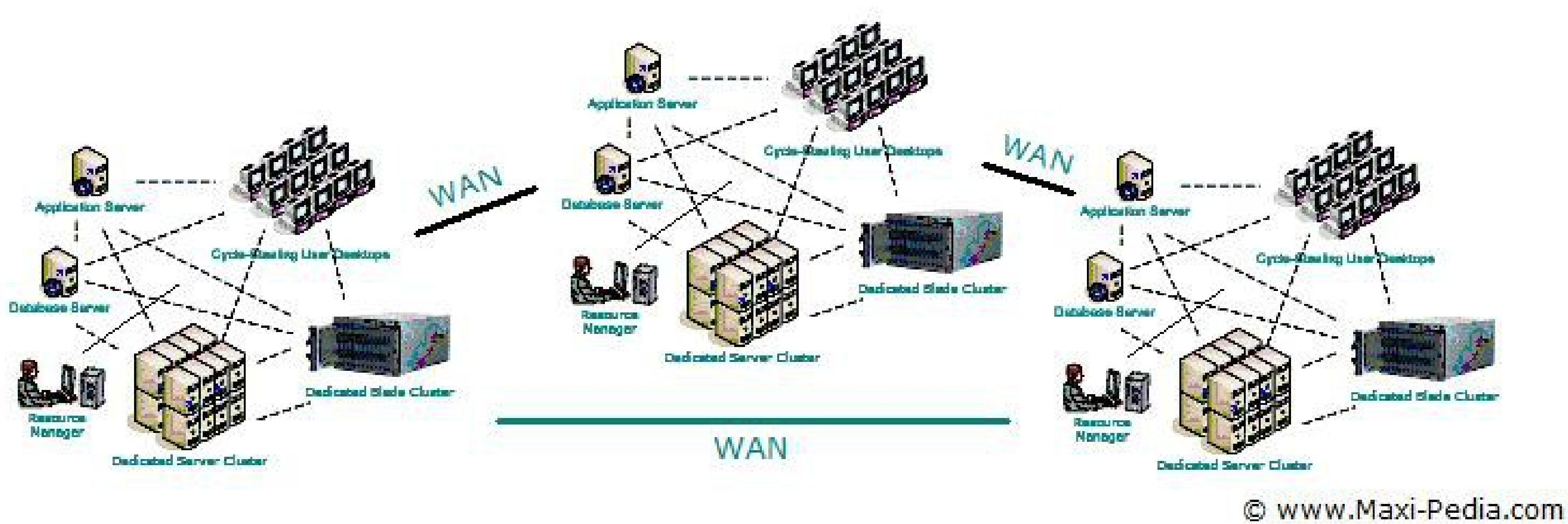
# Cloud Computing

- Homogenous centralized nodes
  - Infrastructure as a Service (IaaS) and Software as as Service (SaaS)
  - Hardware: large datacenters with thousands of servers and a high-speed internet connection
  - Software: virtualized OS and custom software (Docker, etc.)

# Grid Computing

- Heterogenous nodes in disparate physical locations
  - Solving problems or performing tasks of interest to a large number of diverse groups
  - Hardware: different CPUs, GPUs, memory layouts, etc.
  - Software: different OSes, Folding@Home, Condor, GIMPs, etc.



# Aside: linear algebra

- Many scientific phenomena can be modeled as matrix operations
  - Differential equations, mesh simulations, view transforms, etc.
  - Very efficient on vector processors (including GPUs)
  - Data decomposition and SIMD parallelism
  - Dense matrices vs. sparse matrices
  - Popular packages: BLAS, LINPACK, LAPACK

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

# 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 matrix operations no longer work
  - It is a challenge to make sparse operations as efficient as dense operations

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

# HPL benchmark

- HPL: LINPACK-based dense linear algebra benchmark
  - Generates a linear system of equations (answers are all 1.0’s)
  - Distributes data in block-cyclic pattern
  - LU factorization (similar to Gaussian elimination)
  - Backward substitution to solve system
  - Error calculation to verify correctness
  - Compiled on cluster
    - Located in `/shared/apps/hpl-2.1/bin/Linux_PII_CBLAS`

# P3 (OpenMP)

- Similar to HPL benchmark
  1) Random generation of linear system (x is all 1's)
  2) Gaussian elimination
  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)

| | | | | |
|---|---|---|---|---|
| 3.0 | 2.0 | -1.0 | ¦ | 1.0 |
| 2.0 | -2.0 | 4.0 | ¦ | -2.0 |
| -1.0 | 0.5 | -1.0 | ¦ | 0.0 |

Augmented matrix [A | b]

Gaussian elimination

| | | | | |
|---|---|---|---|---|
| 3.0 | 2.0 | -1.0 | ¦ | 1.0 |
| 0.0 | -3.3 | 4.7 | ¦ | -2.7 |
| 0.0 | 0.0 | 0.3 | ¦ | -0.6 |

Upper triangular system

Backward substitution

| | | | | |
|---|---|---|---|---|
| 1.0 | 0.0 | 0.0 | ¦ | 1.0 |
| 0.0 | 1.0 | 0.0 | ¦ | -2.0 |
| 0.0 | 0.0 | 1.0 | ¦ | -2.0 |

Solved system