Massively-Parallel Heterogeneous Computing for Solving Large Problems

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A major paradigm shift

- **In the 20th Century, we were able to understand, design, and manufacture what we can measure**
  - Physical instruments and computing systems allowed us to see farther, capture more, communicate better, …

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- In the 20th Century, we were able to understand, design, and manufacture what we can measure
  - Physical instruments and computing systems allowed us to see farther, capture more, communicate better, understand natural processes, control artificial processes…
- **In the 21st Century, we are able to understand, design, and create what we can compute**
  - Computational models are allowing us to see even farther, going back and forth in time, learn better, test hypothesis that cannot be verified any other way, …

Examples of Paradigm Shift

20th Century

- Small mask patterns
- Electronic microscope and Crystallography with computational image processing
- Anatomic imaging with computational image processing
- Optical telescopes
- Teleconference
- GPS

21st Century

- Optical proximity correction
- Computational microscope with initial conditions from Crystallography
- Metabolic imaging sees disease before visible anatomic change
- Gravitational wave telescopes
- Tele-emersion – augmented reality
- Self-driving cars

What is powering the paradigm shift?

- Large clusters (scale out) allow solving realistic problems
  - 1.5 Peta bytes of DRAM in Illinois Blue Waters
  - E.g., 0.5 Å (0.05 nm) grid spacing is needed for accurate molecular dynamics
    - interesting biological systems have dimensions of mm or larger
    - Thousands of nodes are required to hold and update the grid points.

- Fast nodes (scale up) allow solution at realistic time scales
  - Simulation time steps at femtosecond (10^{-15} second) level needed for accuracy
    - Biological processes take milliseconds or longer
    - Current molecular dynamics simulations progress at about one day for each 100 microseconds of the simulated process.
    - Interesting computational experiments take weeks (used to be months)

What types of applications are demanding computing power today?

- First-principle-based models
  - Problems that we know how to solve accurately but choose not to because it would be "too expensive"
  - High-valued applications with approximations that cause inaccuracies and lost opportunities
  - Medicate imaging, earthquake modeling, weather modeling, astrophysics modeling, precision digital manufacturing, combustion modeling, ….
- Applications that we have failed to program
  - Problems that we just don't know how to solve
  - High-valued applications with no effective computational methods
  - Computer vision, natural language dialogs, stock trading, fraud detection, …

2013: Blue Waters and Titan Computing Systems

System Attribute	NCSA Blue Waters	ORNL Titan
Vendors	Cray/AMD/NVIDIA	Cray/AMD/NVIDIA
Processors	Interlagos/Kepler	Interlagos/Kepler
Total Peak Performance (PF)	12.5	27.1
Total Peak Performance (CPU/GPU)	7.1/5.4	2.6/24.5
Number of CPU Chips	49,504	18,688
Number of GPU Chips	4,224	18,688
Amount of CPU Memory (TB)	1600	584
Interconnect	3D Torus	3D Torus
Amount of On-line Disk Storage (PB)	26	13.6
Sustained Disk Transfer (TB/sec)	>1	0.4-0.7
Amount of Archival Storage	300	15-30
Sustained Tape Transfer (GB/sec)	100	7

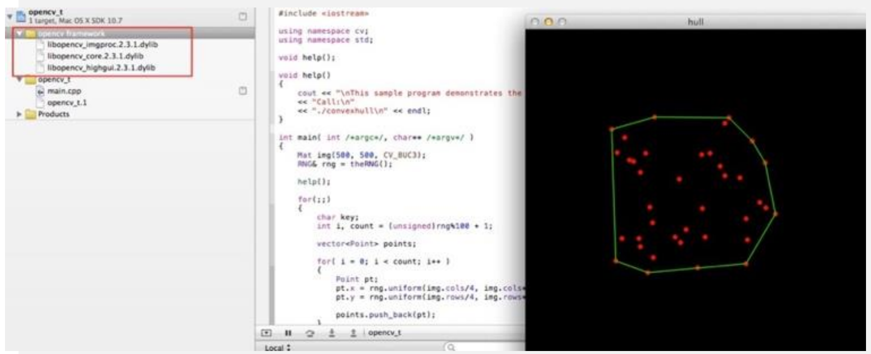
Next Wave of Machines

- To be deployed in 2018-2019
- The NSF leadership machine will be 2-3X of Blue Waters in computing throughput
- This does not increase the problem size much if your algorithm has complexity of $O(N^2)$ or even $O(N \log(N))$
- **The nodes will be limited by the memory bandwidth for most low-complexity algorithms**

Most Blue Waters Job use less than or equal to 4,000 nodes
(1/6 of the machine) today.

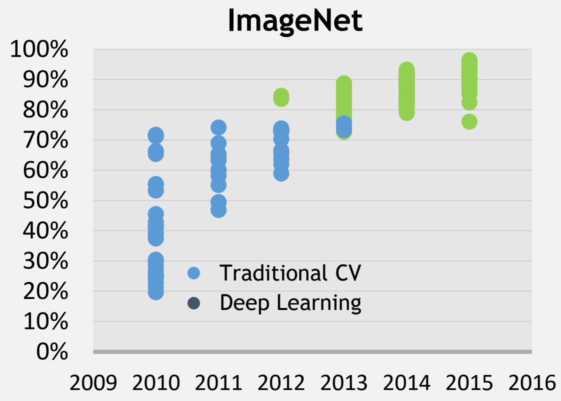
We know what we want but don't know how to build it.

2M training images



Traditional Computer Vision
Experts + Time

Deep Learning Object Detection
DNN + Data + HPC



Deep Learning Achieves
"Superhuman" Results

Slide courtesy of Steve Oberlin, NVIDIA

Some different modalities of Real-world Data

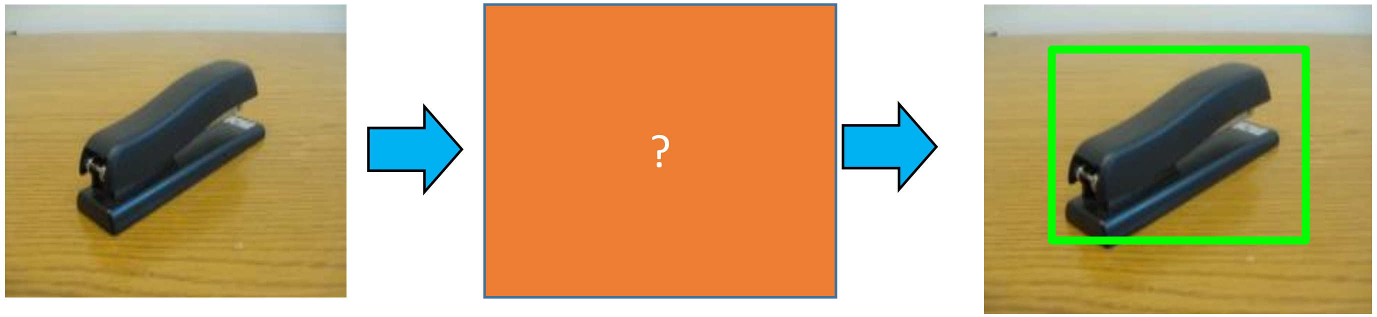
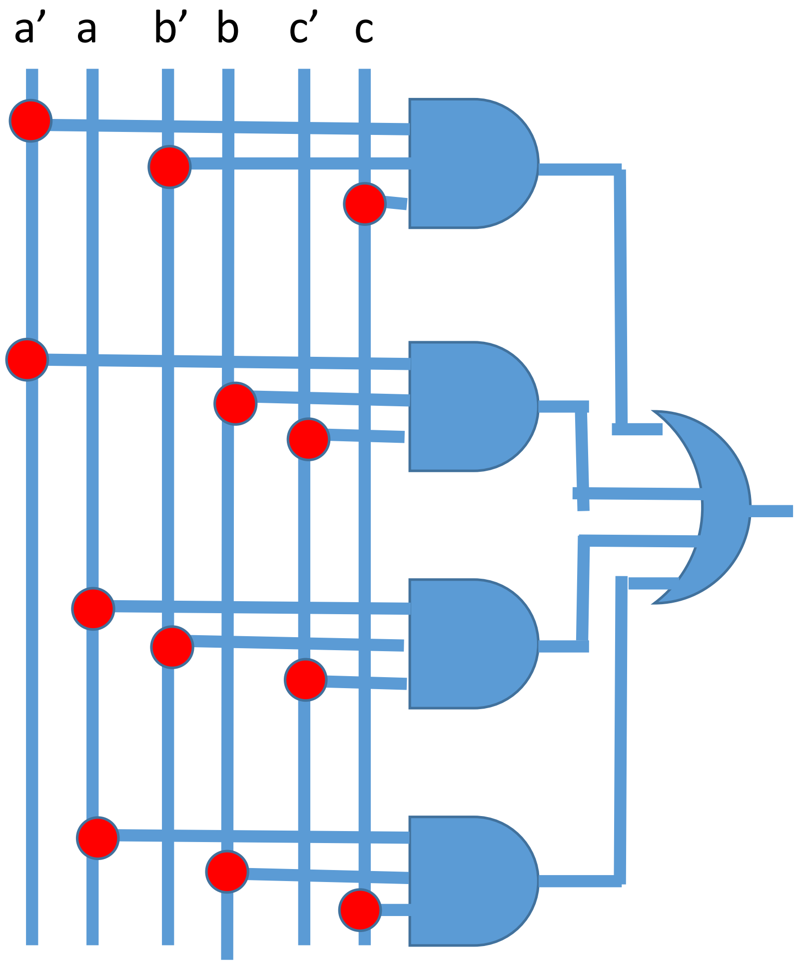


Image | Vision features | Detection

This seems to be a combinational logic design problem.

Combinations Logic Specification – Truth Table

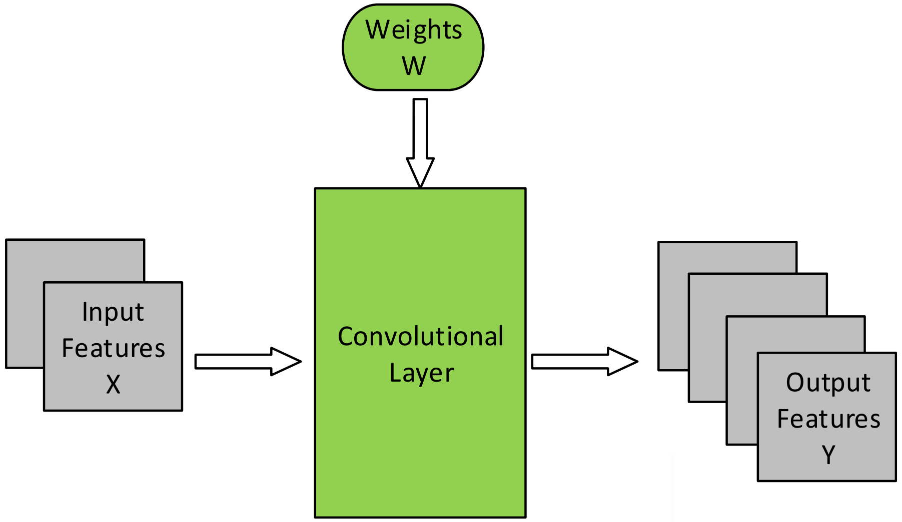
Input			output
a	b	c	
0	0	0	0
0	0	1	1
0	1	0	1
0	1	1	0
1	0	0	1
1	0	1	0
1	1	0	0
1	1	1	1



What if we did not know the truth table?

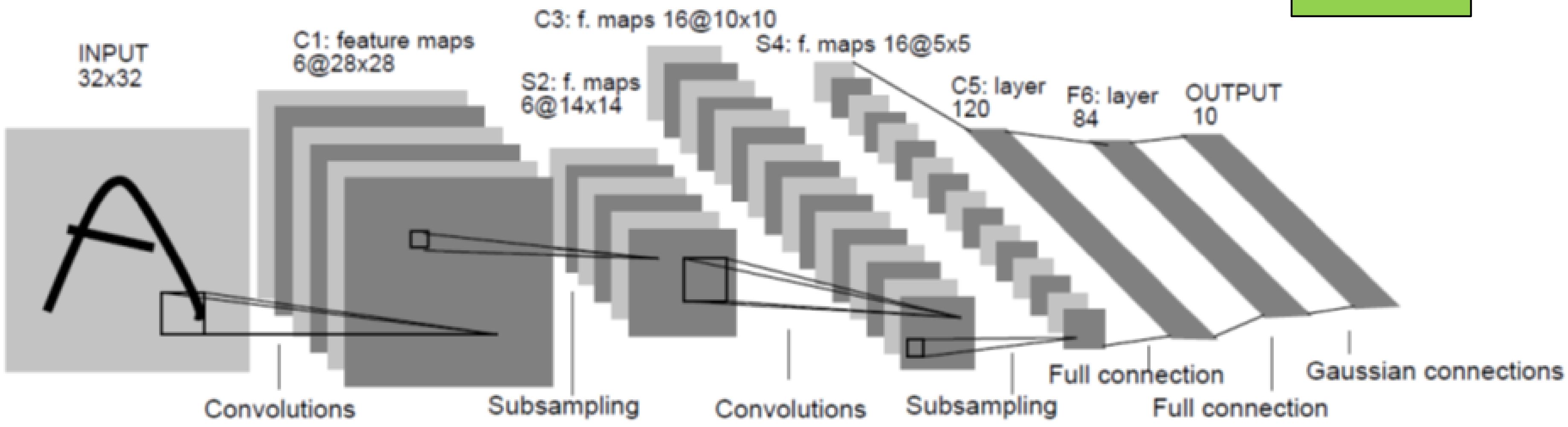
- Look at enough observation data to construct the rules
  - 000 → 0
  - 011 → 0
  - 100 → 1
  - 110 → 0
- If we have enough observational data to cover all input patterns, we can construct the truth table and derive the logic!

LeNet-5, a convolutional neural network for hand-written digit recognition.



This is a 1024*8 bit input, which will have a truth table of 2^{8196} entries

1M training data is approximately 0%



Two Important ML Modalities in Science

- Comparing Theoretical Predictions and Observational Data
  - Using theory to generate training data
  - Use trained model to look for relevant patterns in the observational data
  - Tradeoff training algorithm complexity for reduced data analysis algorithm complexity (LIGO example)

- Using ML to identify the key dimensionalities in simulation or observational data
  - Based on more traditional statistical approaches such as Eigen analysis
  - High algorithm complexity of data analysis

Conclusion and Outlook

- Applications have very large and increasing appetite for more computing power
  - Both larger scale clusters and faster nodes
  - Key to solving large, real world problems

- We can expect only about 2-3X increase in machine capability every 5 years moving forward
  - Low-complexity algorithms will continue to gain importance

- Heterogeneity has become the norm for all hardware systems
  - HPC community are currently seeing about 2-3x application speedup from GPUs
  - Recent positive spiral between deep learning and GPU computing
  - We expect much more heterogeneity in both computing and memory devices in the next generation