# PETASCALE IS THE NEW BLACK

# COMPUTING FOR THE ENDLESS FRONTIER

Niall Gaffney

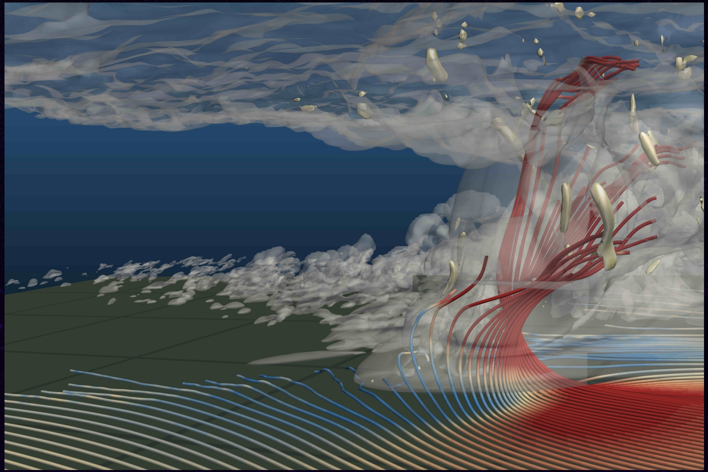
Director of Data Intensive Computing

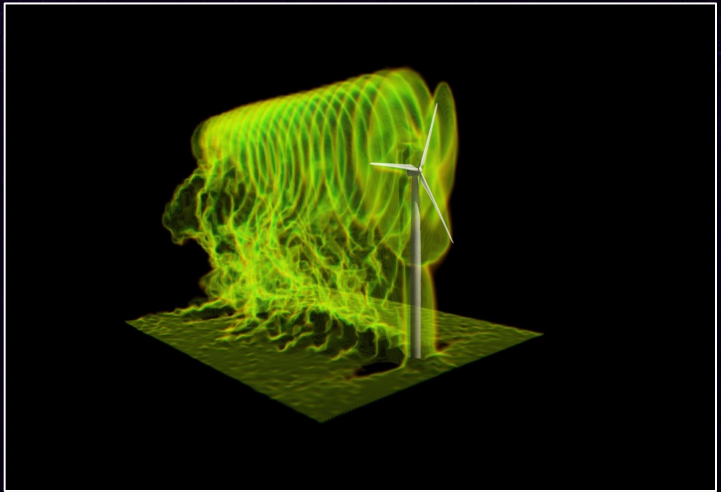
August 2019

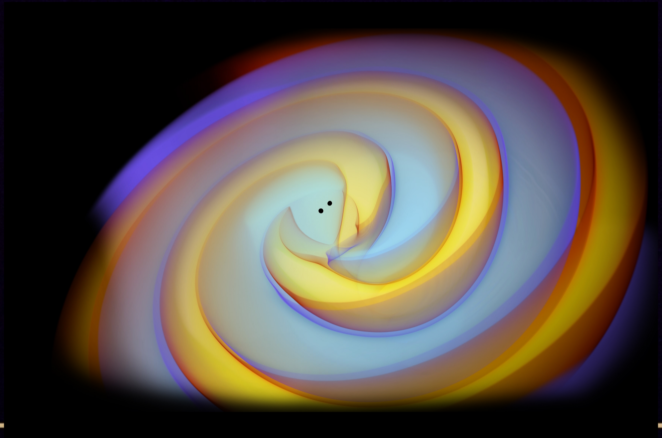
**OR**

**EVERYTHING IS BIGGER IN TEXAS**

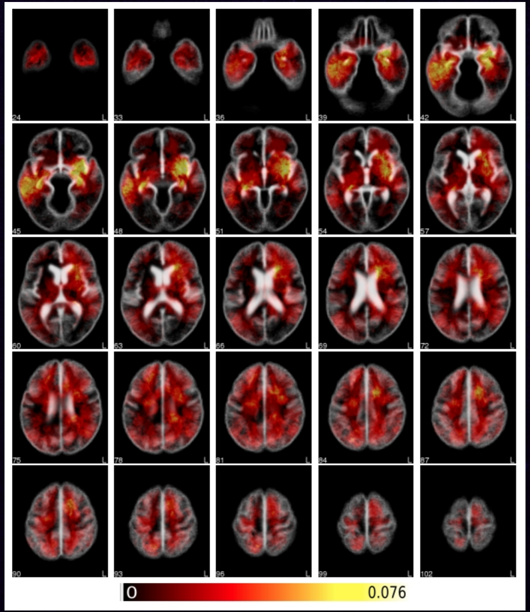
# MOST PEOPLE THINK HPC

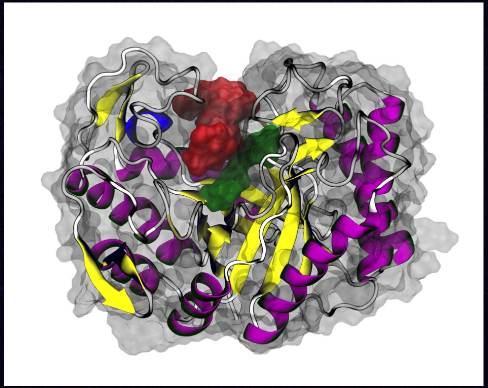






# BUT ITS ALSO….



The first end of Moores Law

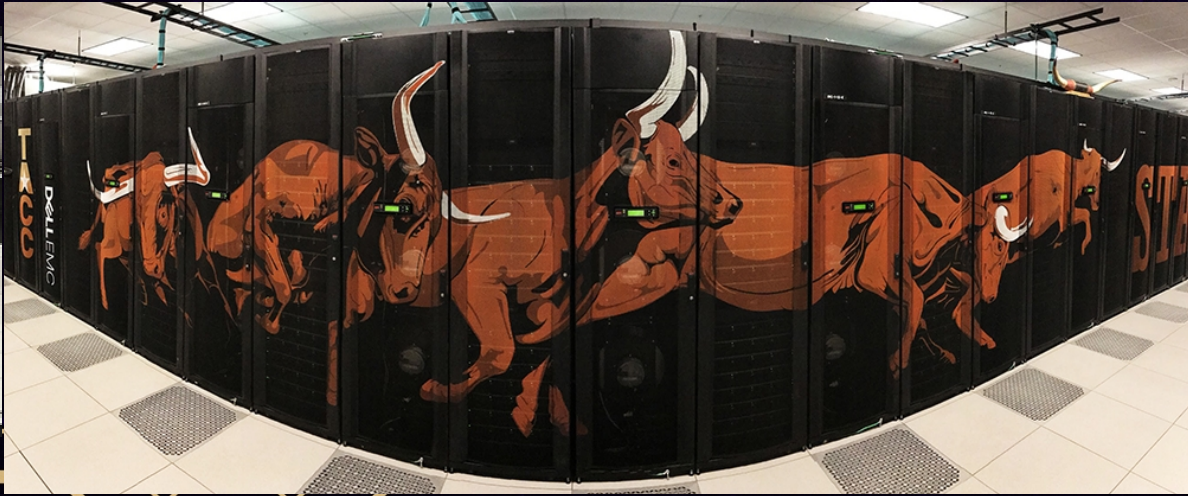
# A BIT OF HISTORY ABOUT PARALLEL COMPUTING
# (AS TOLD BY TACC)

# GROWTH…AND FEWER WHITE BOXES

- 2003 – First Terascale Linux cluster for open science
- 2006 – UT System Partnership to provide Lonestar-3
- **2007 – Ranger is deployed, multicore nodes and InfiniBand fabric**

# NOT AS SIMPLE AT PETASCAL

- 2012,  Stampede replaces Ranger 4000+ nodes each with 16 cores.
- 2015,  Wrangler, first data intensive supercomputer is deployed. 1 TB/s read rate with .5 PB of Flash Storage.
- 2016  Stampede-2 5000+ nodes with 48+ cores per node

# MODERN COMPUTATIONAL SCIENCE

**Simulation**
Computationally query our
*mathematical models* of the world

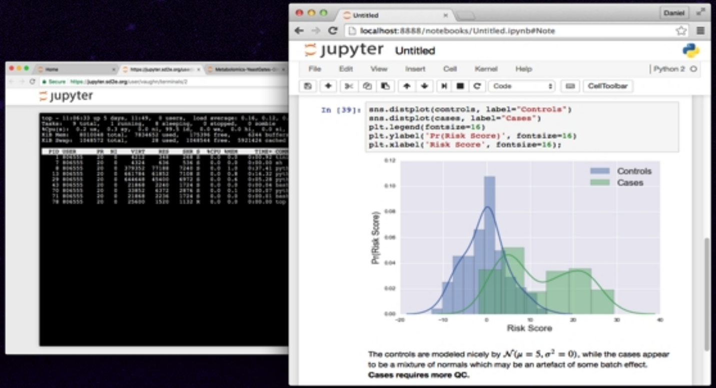
**Machine Learning/AI**
Computationally query our
*data sets*
(depending on technique,
also called deep learning)

**Analytics**
Computationally analyze our
*experiments*
(driven by instruments that produce
lots of digital information)

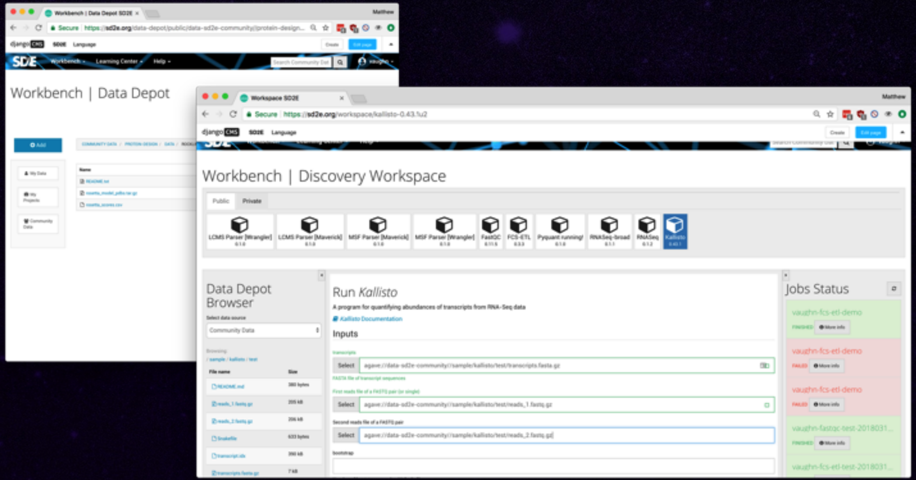
*I would argue that modern science and engineering combine all three*

# HPC DOESN’T LOOK LIKE IT USED TO. . .

**HPC-Enabled Jupyter Notebooks**
*Narrative analytics and exploration environment*




**Web Portal**
*Data management and accessible batch computing*




**Event-driven Data Processing**
*Extensible end-to-end framework to integrate planning, experimentation, validation and analytics*

**From Batch Processing and single simulations of many MPI Tasks –** to that, plus new modes of computing, automated workflows, users who avoid the command line, reproducibility and data reuse, collaboration, end-to-end data management,

- **Simulation** where we have models
- **Machine Learning** where we have data or incomplete models

**And most things are a blend of most of these. . .**

# HPC INTRODUCTION

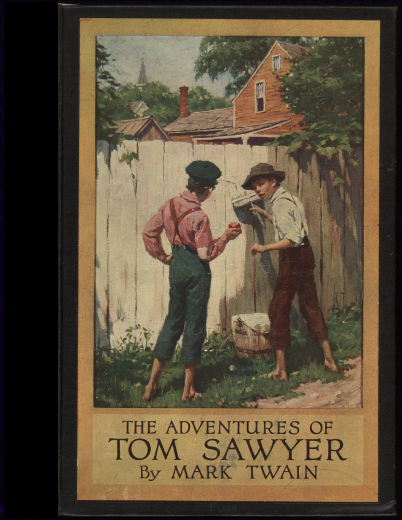
# WHAT IS PARALLEL PROGRAMMING?

More than one paint brush!

Paint the fence faster…

…or paint a bigger fence

**Paint brushes = cores**




The adventures of Tom Sawyer, by Mark Twain [pseud.]
illustrated by Worth Brehm. Adventures of Tom Sawyer. 1910.
In the public domain. From Beinecke Rare Book & Manuscript Library.
http://brbl-dl.library.yale.edu/vufind/Record/3520172?image_id=1010069

# FINE-GRAINED PARALLELISM: VECTORIZATION


C. Holmes 2009
Wikipedia Commons
http://www.flickr.com/photos/inventorchris2/7723117886/

One combine,

multiple rows of wheat

# FINE-GRAINED PARALLELISM: VECTORIZATION

Think tight, long inner loops with a few familiar array calculations:

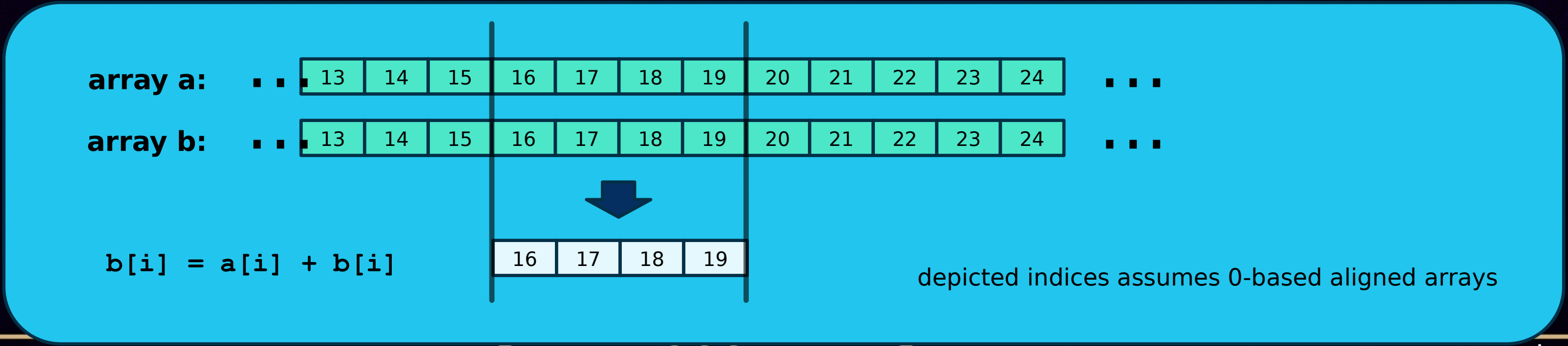
C. Holmes 2009
Wikipedia Commons
http://www.flickr.com/photos/inventorchris2/7723117886/

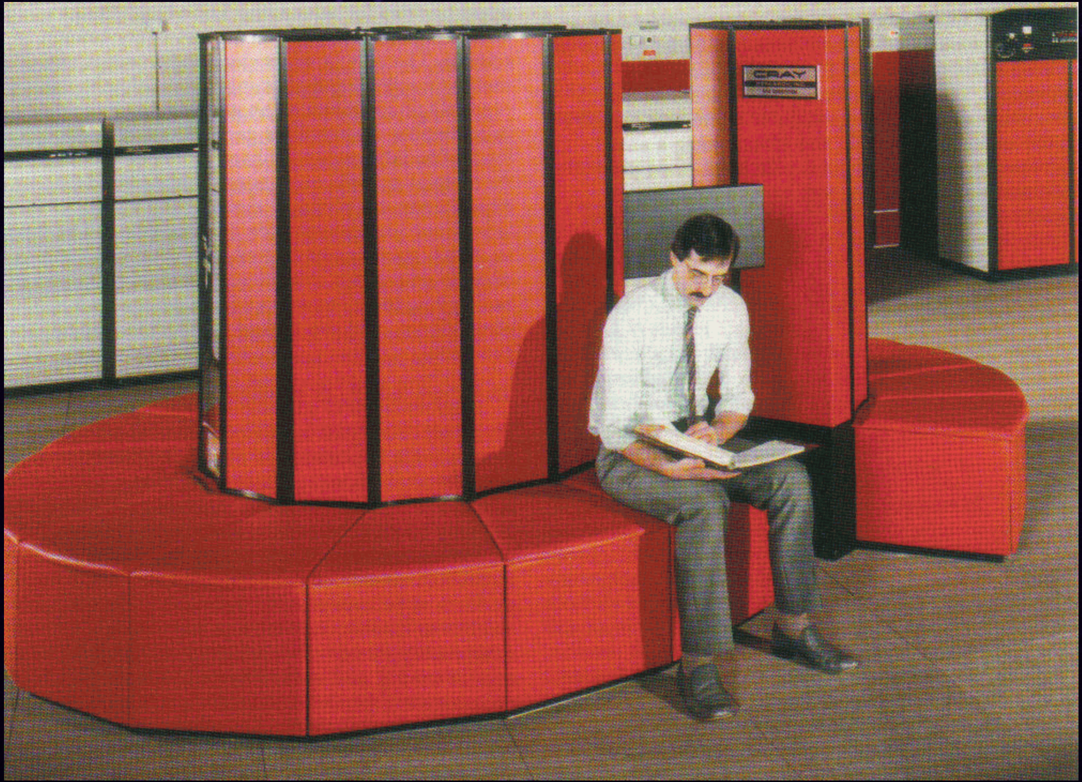
```
/* C-style loop */

for ( int i=0; i<n; i++ )
     c[i] = a[i] + b[i];

------

c = a + b   !Fortran arrays
```

# VECTORIZATION:

Each core has multiple vector units

- One supports floating point addition, the other multiplication
- Each can produce up to multiple double precision results/cycle



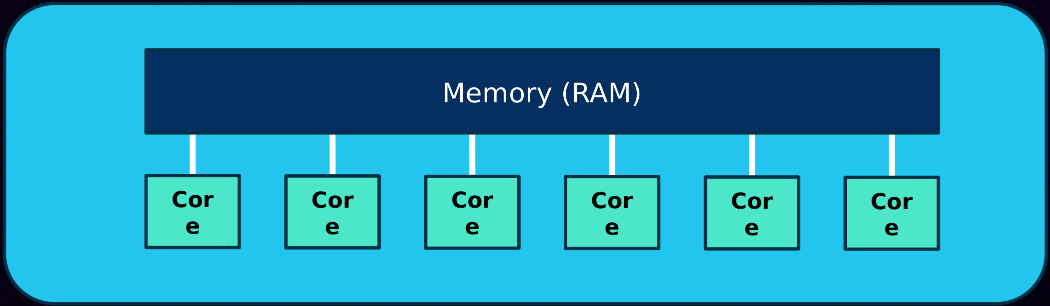



http://www.chilton-computing.org.uk/ccd/literature/serc_annual_reports/serc_86-87.htm

# SHARED MEMORY

- All cores share a common pool of memory (RAM)
- The programming challenge is coordination: how to avoid competing for access to the same puzzle pieces (memory)
- Principal programming model: OpenMP
- A **single executable** spawns independent threads and manages threads' access to data

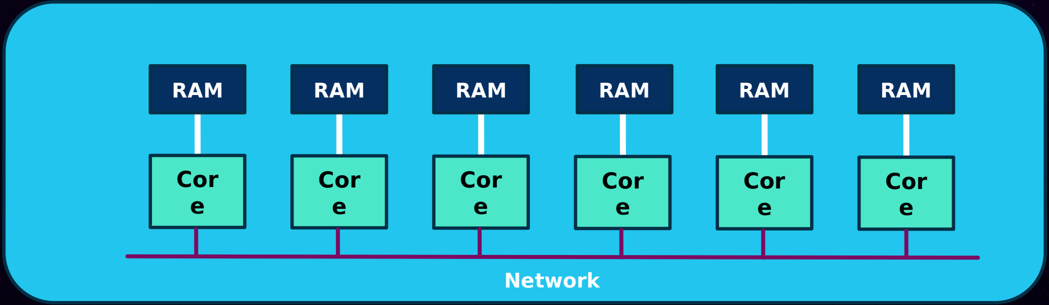
Octahedron80 2007
Wikipedia Commons
http://commons.wikimedia.org/wiki/File:Jigsaw_pieces_with_border.jpg



# DISTRIBUTED MEMORY

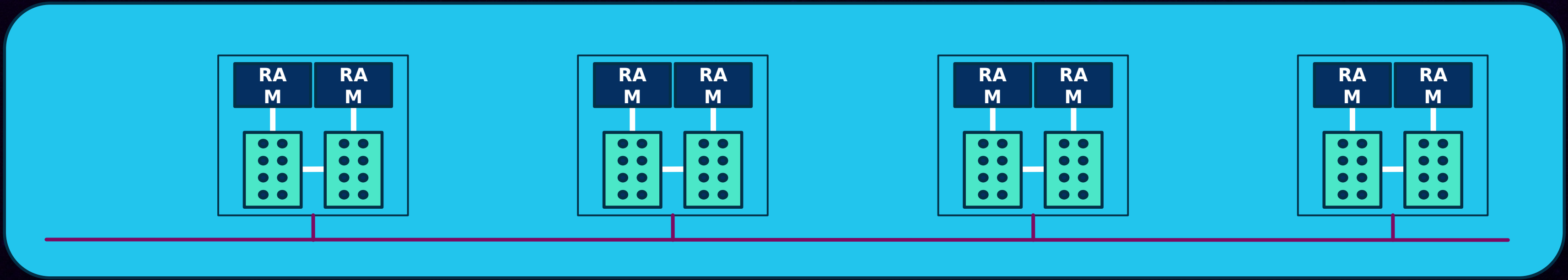
- Each core* has its own memory (RAM), inaccessible to other cores
- The programming challenge is communication: how to share puzzle pieces (data)
- Principal programming model is MPI (Message Passing Interface)
- Every assigned core runs a separate copy of the same executable -- a “rank aware” task

Octahedron80 2007
Wikipedia Commons
http://commons.wikimedia.org/wiki/File:Jigsaw_pieces_with_border.jpg



# HYBRID ARCHITECTURE

- Most large clusters are hybrids of these models
  - Each node is a multi-core shared memory computer running its own (Linux) operating system
  - Many such nodes connected in distributed configuration
  - Each core sees only the memory on its own node!

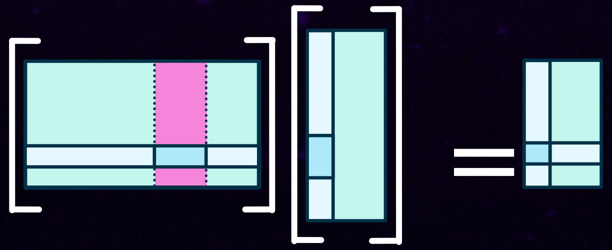


# FRONTERA: #5 IN THE WORLD


# LINEAR ALGEBRA KERNELS

Off-the-shelf optimization and parallelism from mature, robust libraries; e.g.

- Intel Math Kernel Library (MKL) -- robust support for MIC
- PETSc – dense and sparse object-oriented solvers
- FFTW3 – Distributed fourier transform mechanism
- Lots of others (I'm probably skipping your favorite...)

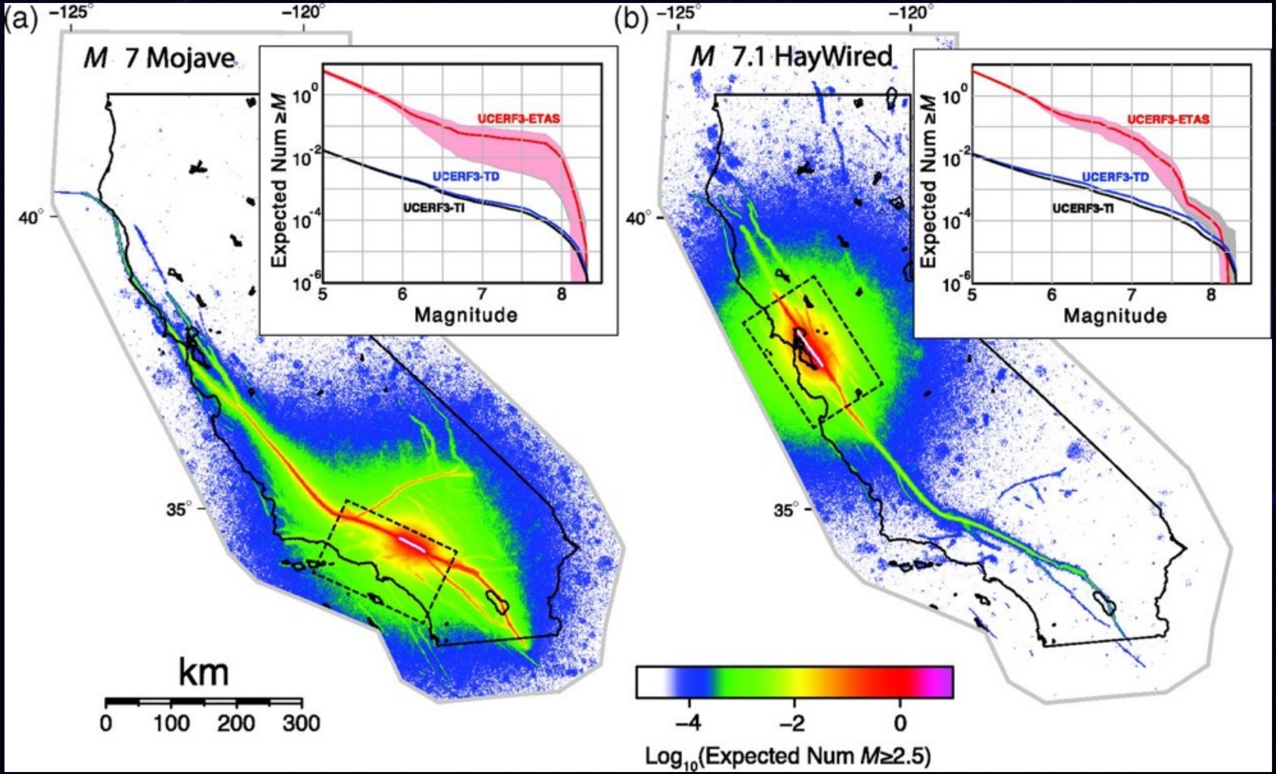


# M87

- First image of the shadow cast by the blackhole at the center of galaxy Messier 87 collected by the Event Horizon Telescope
  - Global scale radio telescope observations
  - Petascale compute just to make image
- Predictions made about what to expect using NSF supercomputers including Stampede 2 by Ramesh Narayan’s team at Harvard (and others).
  - Simulated the black hole system with different physics models (General Relativity vs. alternatives)
  - Simulated appearance of each to compare to observed model to test theory

TACC Press Release

# AFTERSHOCK FORECASTING



# HPC AND “BIG DATA”

Enter Machine Learning

# ARTIFICIAL INTELLIGENCE SCOPE

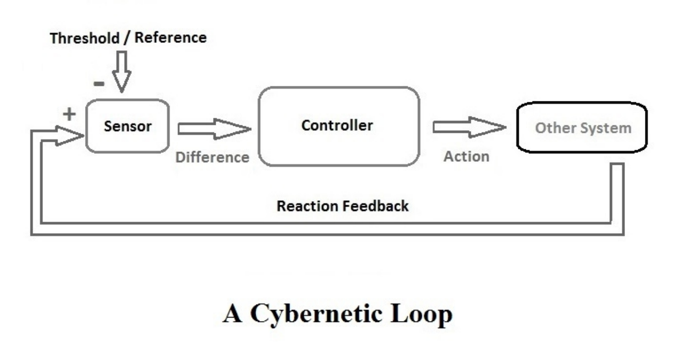
*“The true challenge to artificial intelligence proved to be solving **the tasks that are easy for people to perform but hard for people to describe formally**—problems that we solve intuitively, that feel automatic, like recognizing spoken words or faces in images.”*

— *Ian Goodfellow, Yoshua Bengio, Aaron Courville*

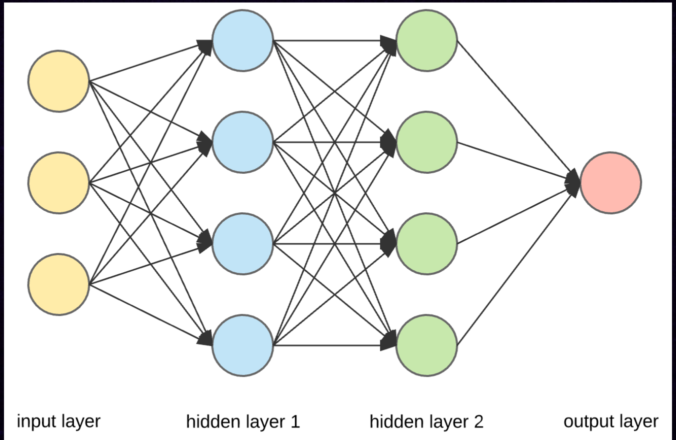
# DEEP LEARNING OVERVIEW

- Deep learning is a class of machine learning algorithms in which multiple layers of nonlinear processing units are used for feature extraction and transformation, with each successive layer taking the output from the previous layer as input
  - Its what you have to do when you don’t have reliable equations to model a system
  - Sometimes its better than when you do
  - And sometimes, you need both

# HISTORY




- 60s — Cybernetics
- 90s — Connectionism + Neural Networks
- 10s — Deep Learning
  - Two key factors for the on-going renaissance
    - Computing capabilities
    - Large datasets on high throughput I/O systems



# DEEP LEARNING APPLICATIONS



credits: https://upload.wikimedia.org/wikipedia/commons/1/1b/Google%27s_Lexus_RX_450h_Self-Driving_Car.jpg
credits: https://upload.wikimedia.org/wikipedia/commons/thumb/c/cd/Uber_OTTO_autonomous_driving_truck.jpg/640px-Uber_OTTO_autonomous_driving_truck.jpg

# DEEP LEARNING APPLICATIONS

- The GO game


credits: https://c1.staticflickr.com/2/1626/25708381781_eee5664c65_b.jpg

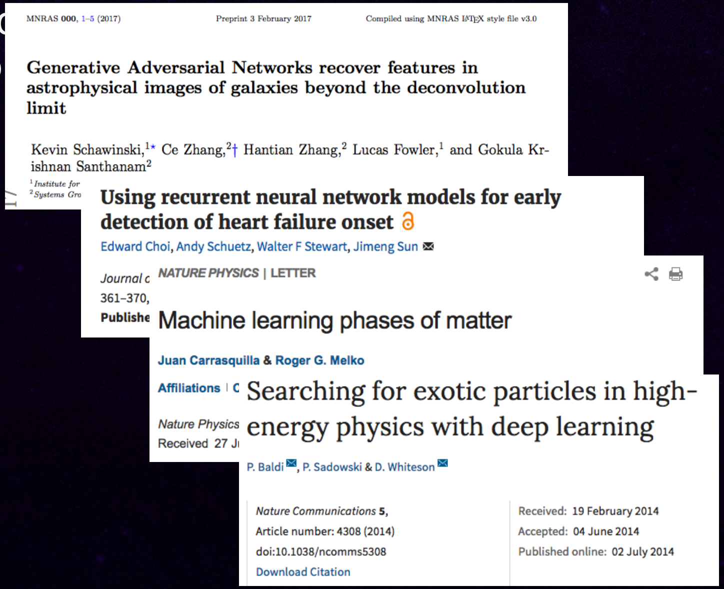
# DEEP LEARNING APPLICATIONS


- DOTA

credits: https://openai.com/five/

# DEEP LEARNING APPLICATIONS

- Many scientists are exploring and adopting d
data science methodology to tackle their do
challenge
  - Astronomy
  - Drug discovery
  - Disease diagnosis
  - Molecular dynamics
  - Neurology
  - Particle physics
  - Social science


MNRAS 000, 1–5 (2017) Preprint 3 February 2017 Compiled using MNRAS LaTeX style file v3.0

**Generative Adversarial Networks recover features in astrophysical images of galaxies beyond the deconvolution limit**

Kevin Schawinski,[1*] Ce Zhang,[2†] Hantian Zhang,[2] Lucas Fowler,[1] and Gokula Krishnan Santhanam[2]

**Using recurrent neural network models for early detection of heart failure onset**

Edward Choi, Andy Schuetz, Walter F Stewart, Jimeng Sun

NATURE PHYSICS | LETTER

Machine learning phases of matter

Juan Carrasquilla & Roger G. Melko

Searching for exotic particles in high-energy physics with deep learning

P. Baldi, P. Sadowski & D. Whiteson

Nature Communications 5, Article number: 4308 (2014) doi:10.1038/ncomms5308 Download Citation

Received: 19 February 2014 Accepted: 04 June 2014 Published online: 02 July 2014

# DL IN SCIENCE

ml4science

8:50-9:06 Data-driven methods for the discovery of governing equations

J. Nathan Kutz, UW

9:38-9:54 Data Driven Discretization for Partial Differential Equations

Stephan Hoyer, Google Research

9:54-10:10 Solving Astrophysical PDEs with Deep Neural Networks and TensorFlow

Milos Milosavljevic, The University of Texas at Austin

10:35-10:51 Machine learning for lattice gauge theory

Phiala Shanahan, MIT

10:51-11:07 Physics informed Machine Learning

Guofei Pang, Brown

11:07-11:23 Machine learning in high-energy particle physics experiments, from simulation, through reconstruction to physics analysis

Heather Gray, UC Berkeley/LBNL

11:39-11:55 Physics Constrained Fluid Flow Prediction using Lyapunov's Method

Ben Erichson, UC Berkeley

11:55 - 12:11 Cosmology for Machine Learning

Uros Seljak, UC Berkeley/LBNL

# DL IN SCIENCE

1:16-1:32 Flow-based generative models for lattice field theory

Tej Kanwar, MIT

1:32-1:48 Putting Non-Euclidean Geometry to Work in ML: Hyperbolic and Product Manifold Embeddings

Frederic Sala, Stanford

1:48-2:04 Deducing Inference from Hyperspectral Imaging of Materials Using Deep Recurrent Neural Networks

Joshua Agar, Lehigh University

2:04-2:20 Improved learning for materials and chemical structures through symmetry, hierarchy and similarity

Bert de Jong, LBNL

2:20 - 2:36 CosmoGAN: Towards a cosmology emulator using Generative Adversarial Networks

Mustafa Mustafa, LBNL

2:36 - 2:52 Hybrid Physical - Deep Learning Models for Astronomical Inverse Problems

François Lanusse, UC Berkeley

4:03-4:19 Reinforcement Learning for Materials Synthesis

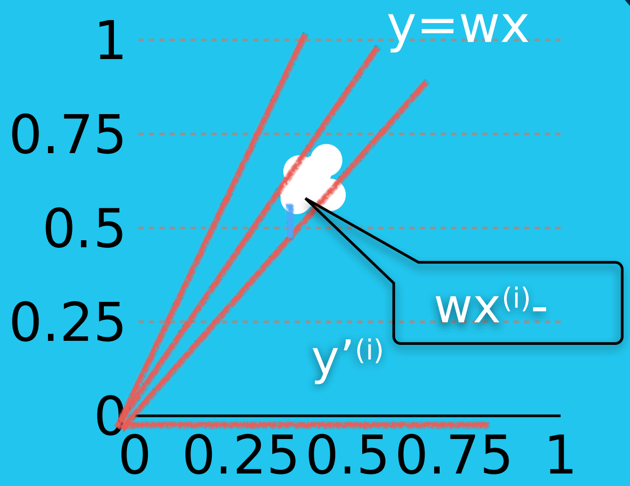
Rama Vasudevan, Oak Ridge National Laboratory

ml4science

# LINEAR REGRESSION

- Example: Predicting house price with square footage

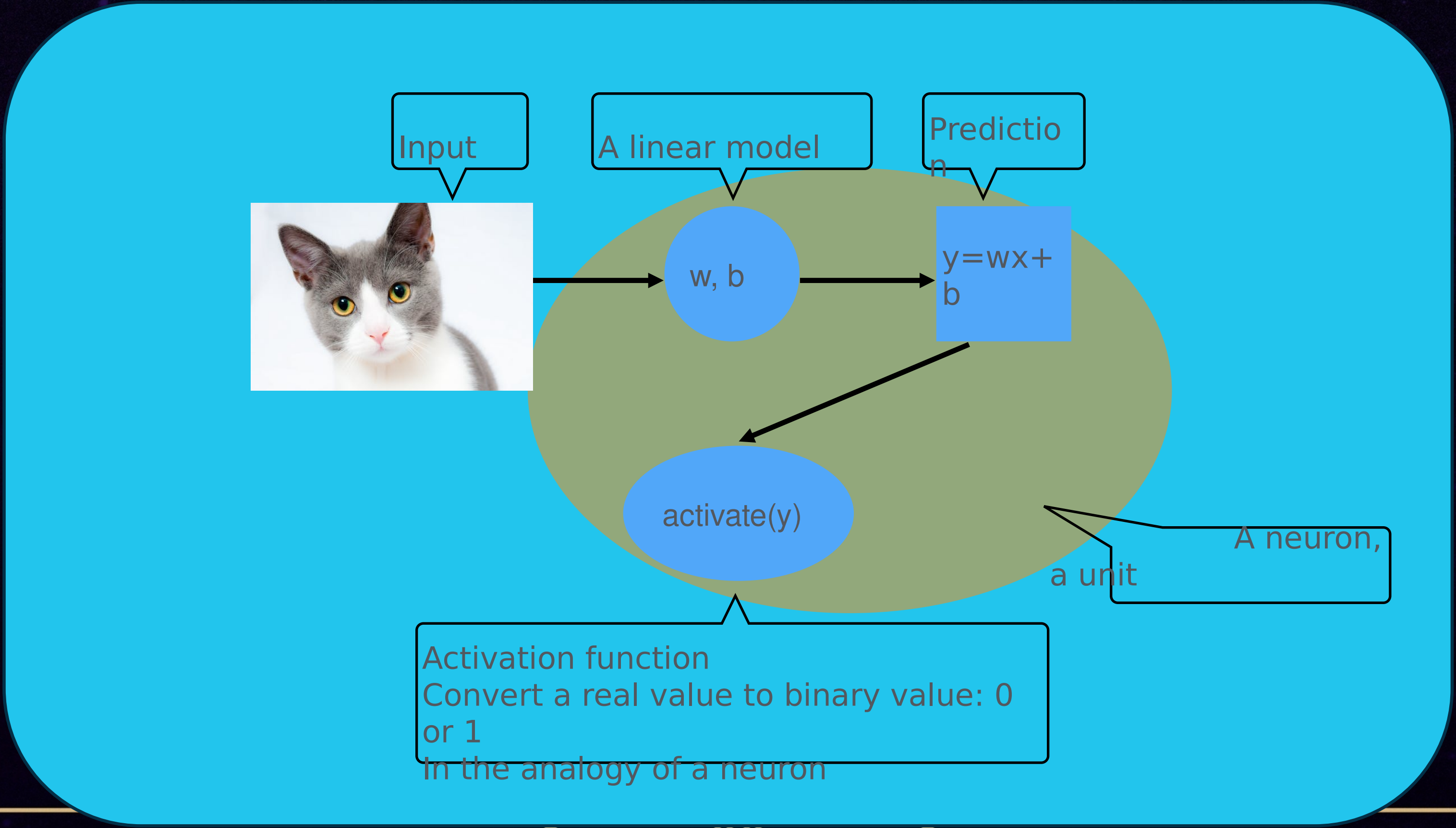
| ID | $x^{(i)}$, sqft/$10^4$ | $y'^{(i)}$, price/$10^6$ |
|---|---|---|
| 1 | 0.3801 | 0.58 |
| 2 | 0.4271 | 0.5975 |
| 3 | 0.4580 | 0.588 |
| 4 | 0.3780 | 0.6 |
| 5 | 0.3890 | 0.623 |
| 6 | 0.4250 | 0.65 |
| 7 | 0.4500 | 0.68 |
| 8 | 0.3867 | 0.65 |




Train a function $y=w*x$ to minimize

Loss $=1/2 * \sum(wx^{(i)}-y'^{(i)})^2$

# FROM LINEAR REGRESSION TO NEURAL NETWORK



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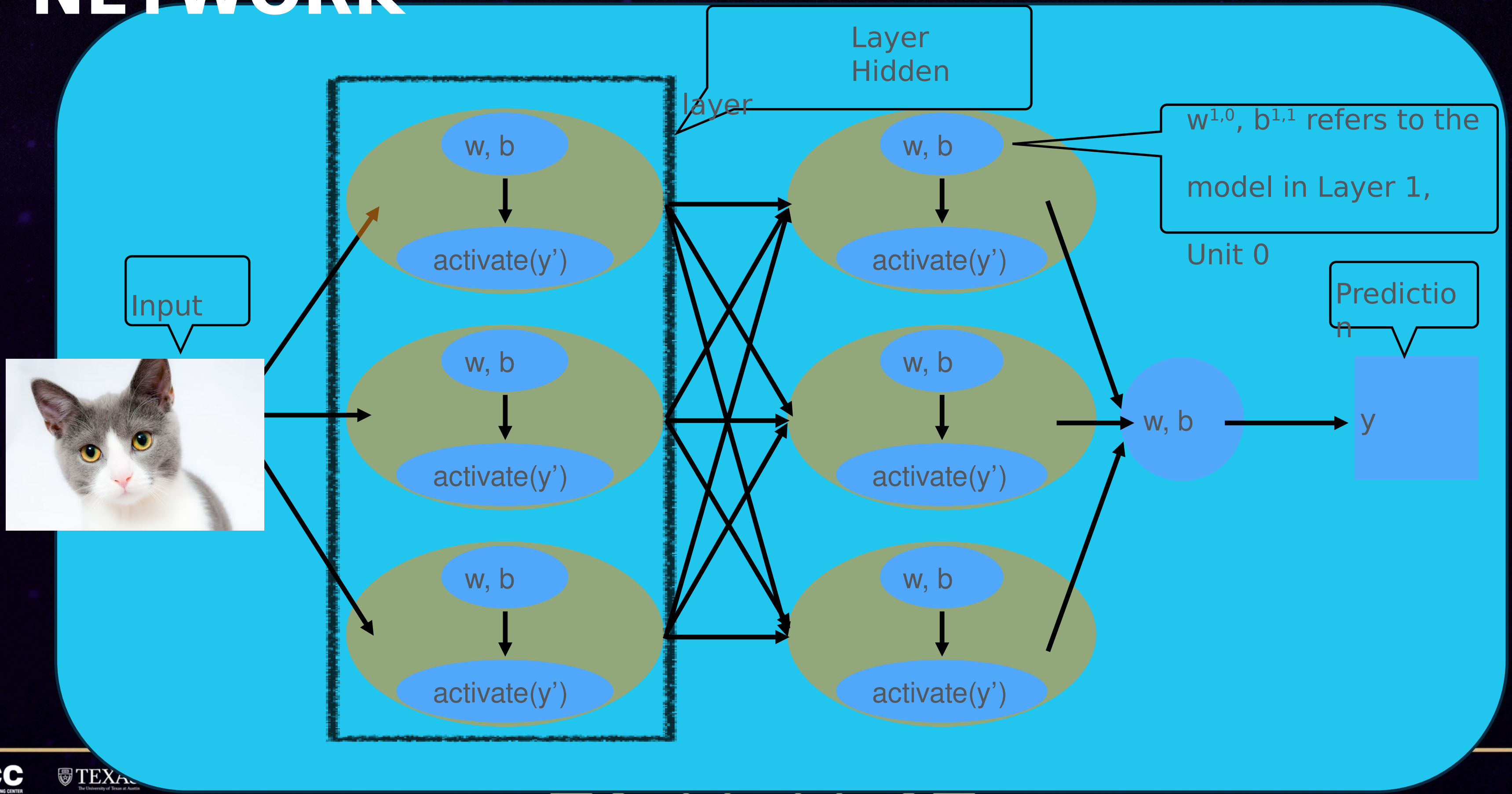
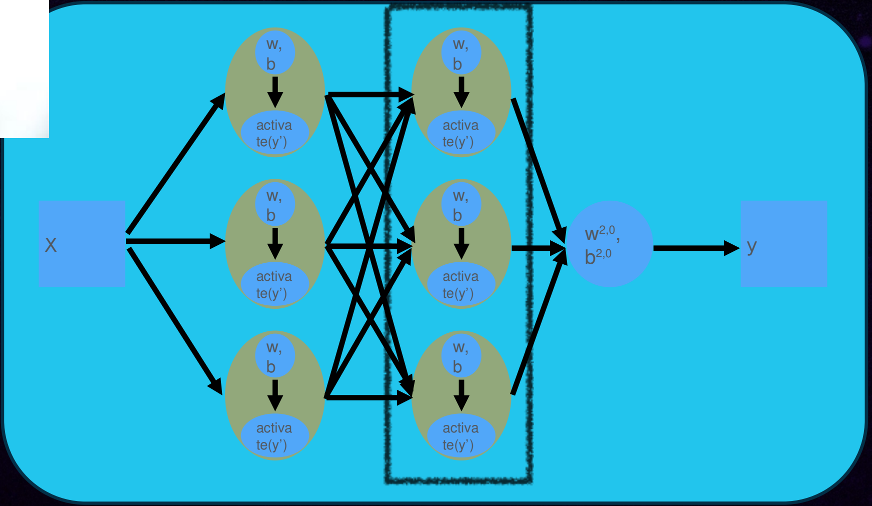


# FROM LINEAR REGRESSION TO NEURAL NETWORK

CAT

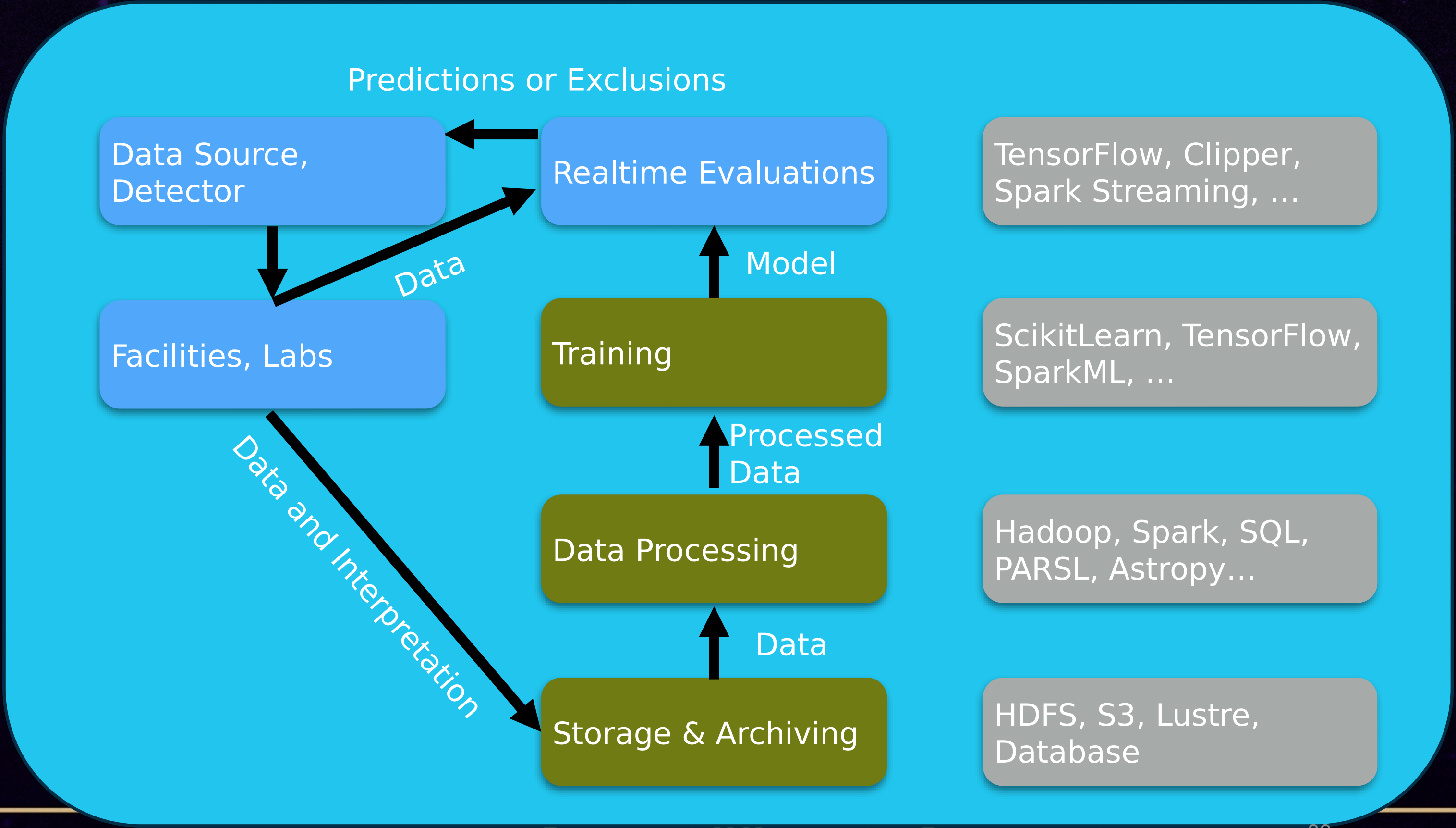
DOG

HOTDOG

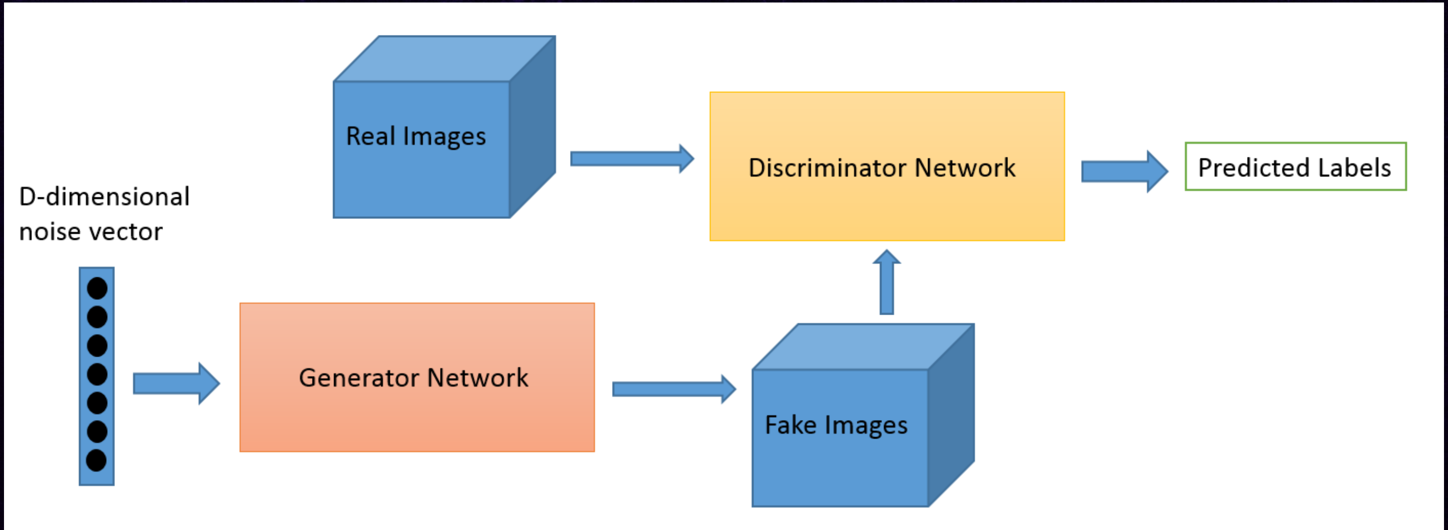



- Now we have labeled data
- We can calculate y and the error with label y’
- We can then update $w^{2,0}$

# DATA-DRIVEN DECISION MAKING PIPELINE

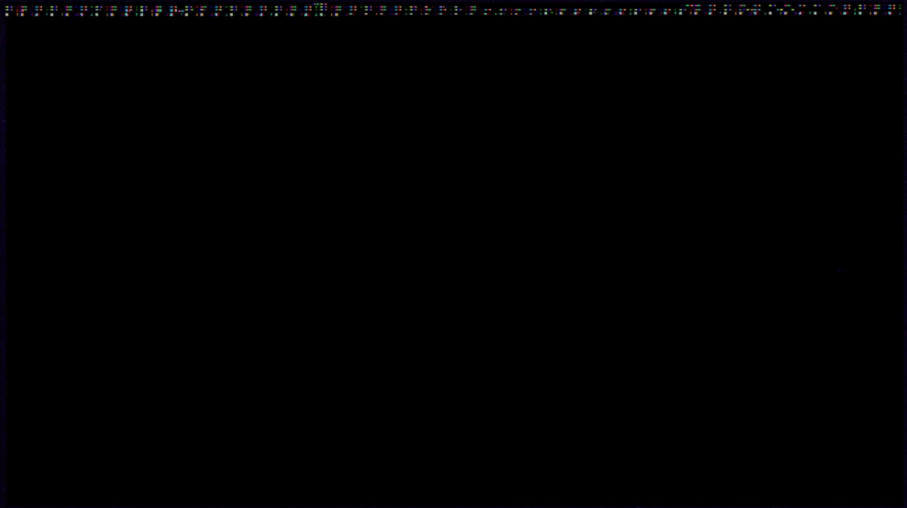


# GENERATIVE ADVERSARIAL NETWORK



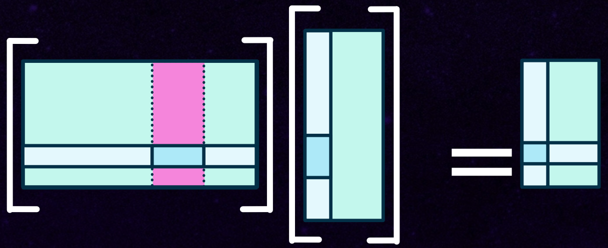

Courtesy image from O'Reilly

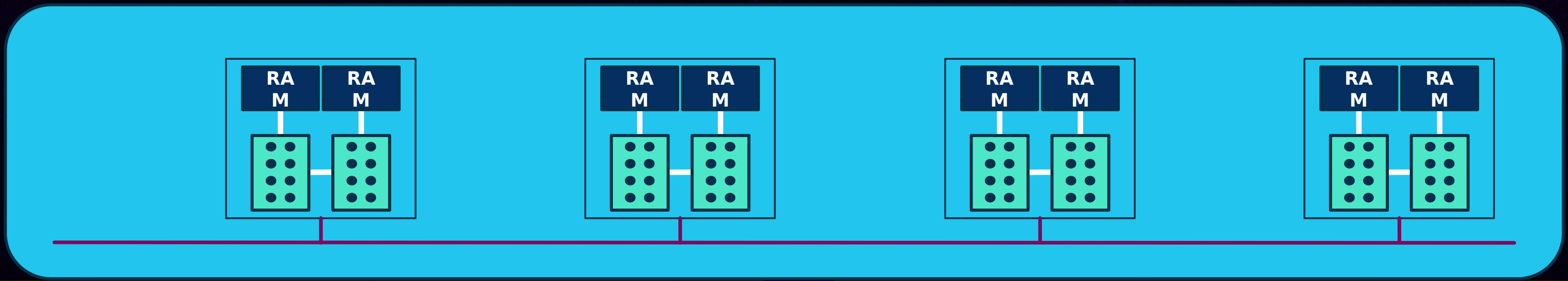
# GENERATIVE ADVERSARIAL NETWORK



# ISN'T THIS THE SAME THING AS HPC?

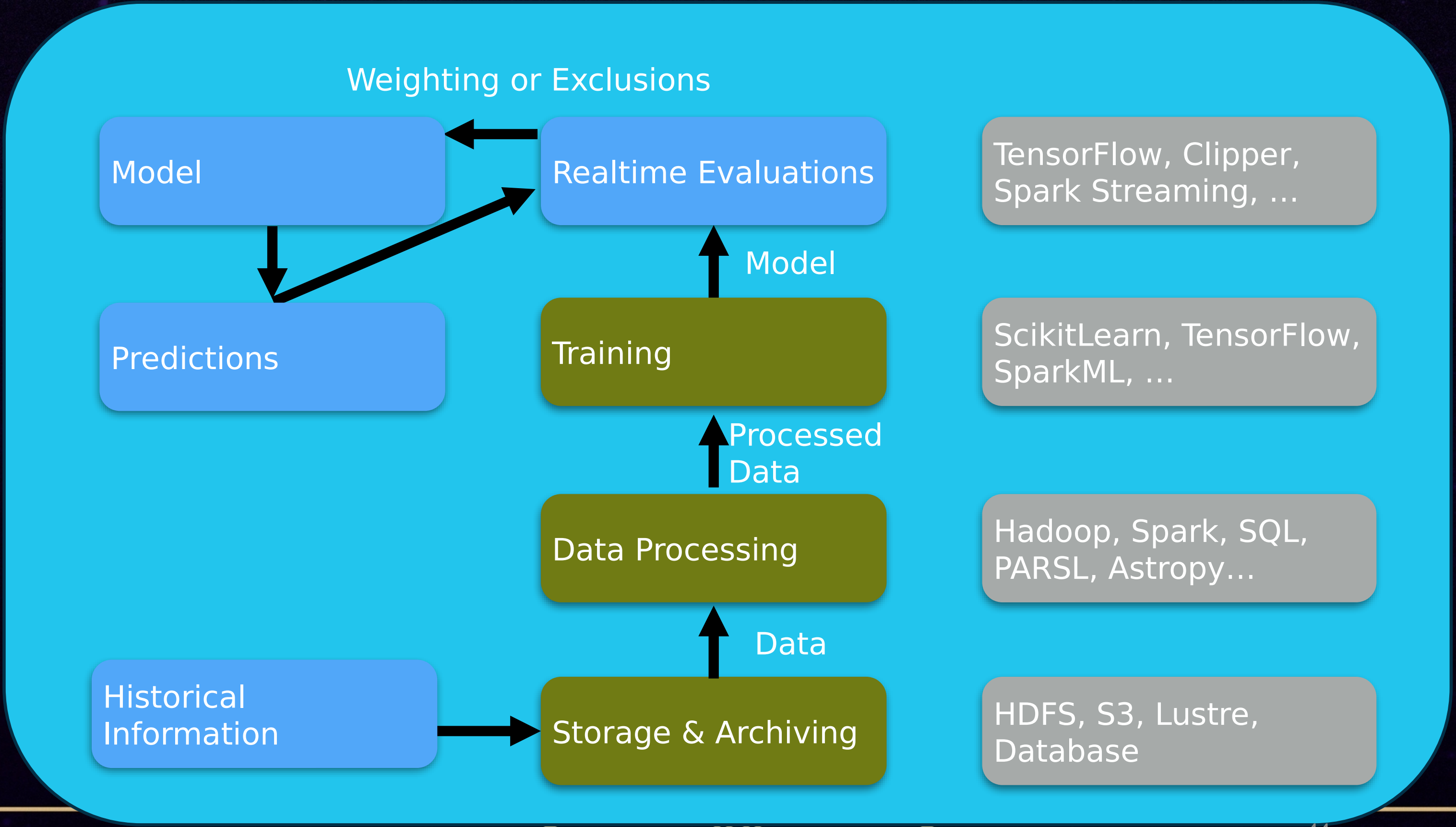
- Optimized for low precision not high precision computations.
- GPUs, TPUs, New Intel chips
  - Tensorflow
  - PyTorch
- Some Message Passing Architectures





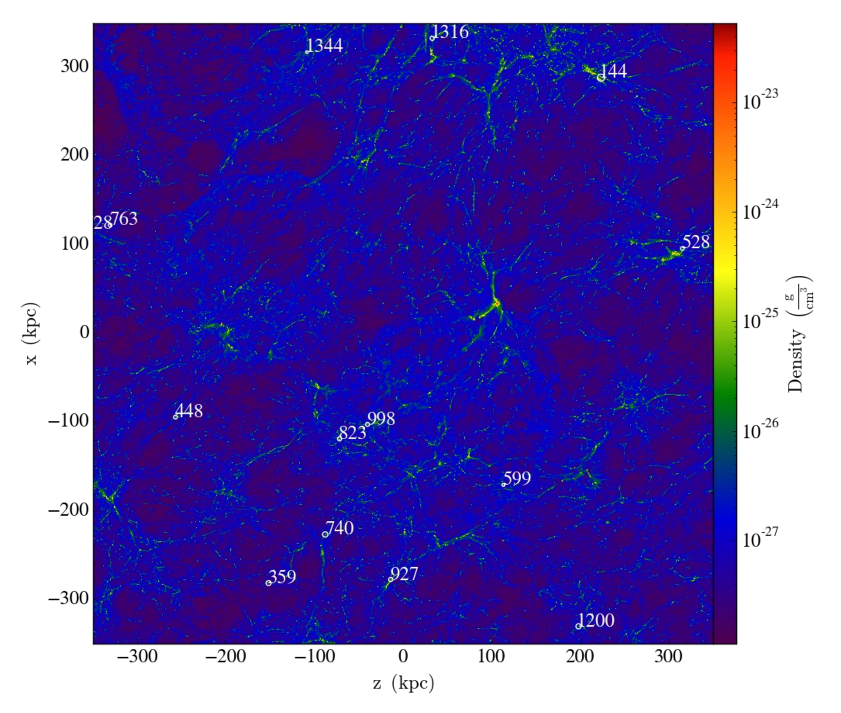
# “BUT I KNOW MY MODELS EQUATIONS OF STATE”

# DATA-DRIVEN MODEL INTERPRETATION

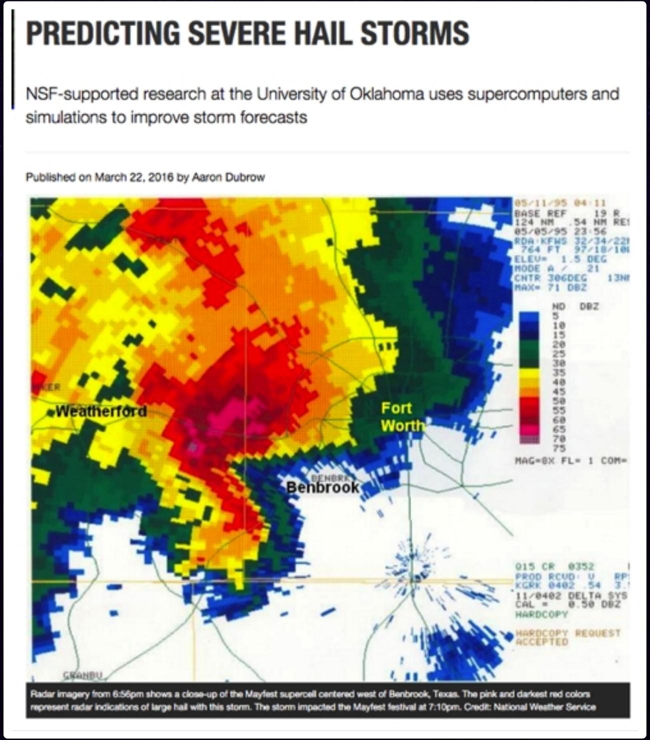


# COSMOLOGICAL STRUCTURE VISUALIZATION

- Initial dataset: 50TB Blue Waters
- Feature detection and projection
- Finding the needle in the simulated universal haystack (where more detailed exploration is needed)



# EXTREME WEATHER FORECASTING



## PREDICTING SEVERE HAIL STORMS

NSF-supported research at the University of Oklahoma uses supercomputers and simulations to improve storm forecasts

Published on March 22, 2016 by Aaron Dubrow



Radar imagery from 6:56pm shows a close-up of the Mayfest supercell centered west of Benbrook, Texas. The pink and darkest red colors represent radar indications of large hail with this storm. The storm impacted the Mayfest festival at 7:10pm. Credit: National Weather Service

University of Oklahoma researchers improving prediction of severe hail storms

- Combined traditional ensemble weather simulation output with machine learning classification based on observed historical weather data
- Reduced ensemble outputs to those that were realistic
- Improved effective prediction timescales from 2 to 24 hours

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(depending on technique,
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*I would argue that modern science and engineering combine all three*


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