

High Performance Computing

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Logistics

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- Class: Mon, Wed: 4 – 5:15
- Drop date: 01/19/2016
- Questions / Discussions:
 - (Questions, project discussions, assignments...)
- Office Hours: Send an email to ashish.sharma@emory.edu
 - Office: #573, Psychology Building
- Grading:

• Class Participation:	30%
• Assignments:	30%
• Final Project:	40%
- Lecture Slides, Readings etc., will be posted on github
 - Lookout for an announcement on slack

Class Participation

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- 15min presentations on current state of HPC
[Class reading list & your own research]
- Guest Lectures on HPC applications: **Varies**
- Occasional 5min quizzes
- Active Participation:
 - Attend regularly
 - Participate (Class & Slack)
 - Start early with project

Academic Integrity

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- Review the Emory Honor Code
- Penalty for academic dishonesty is a 0 on the assignment and half of your class participation grade. **For all involved.**
- It is your responsibility to protect your work
- All assignments are individual unless prior permission is explicitly granted. Any evidence of cooperation or plagiarism will be considered academic dishonesty
 - You are allowed to discuss and seek help on systems, installation, getting-started issues. **When in doubt ASK ME**
 1. Only from fellow classmates (~~Stackoverflow, Quora, ...~~)
 2. Suggest using slack for this, so that others can benefit from this (also counts towards class participation grade)

Acknowledgements

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Similar courses that were helpful in preparing these lectures

- G63.2011.002/G22.2945.001: High Performance Scientific Computing
 - Marsha Berger & Andreas Klöckner – NYU
- CS 759: High Performance Computing for Engineering Applications
 - Dan Negrut – Univ. of Wisconsin
- CS267: Applications of Parallel Computers
 - Jim Demmel – Berkeley
- CS525: Parallel Computing
 - Ananth Grama – Purdue
- Seminar Series on High Performance Computing at The National Institute for Computational Science, University of Tennessee, Knoxville

Textbooks

- Introduction to Parallel Computing by Grama, Gupta, Kumar, Karypis
- Introduction to High-Performance Scientific Computing by Eijkhout

Introductions

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- Name:
- Program:
- Describe what you expect to gain from this course:

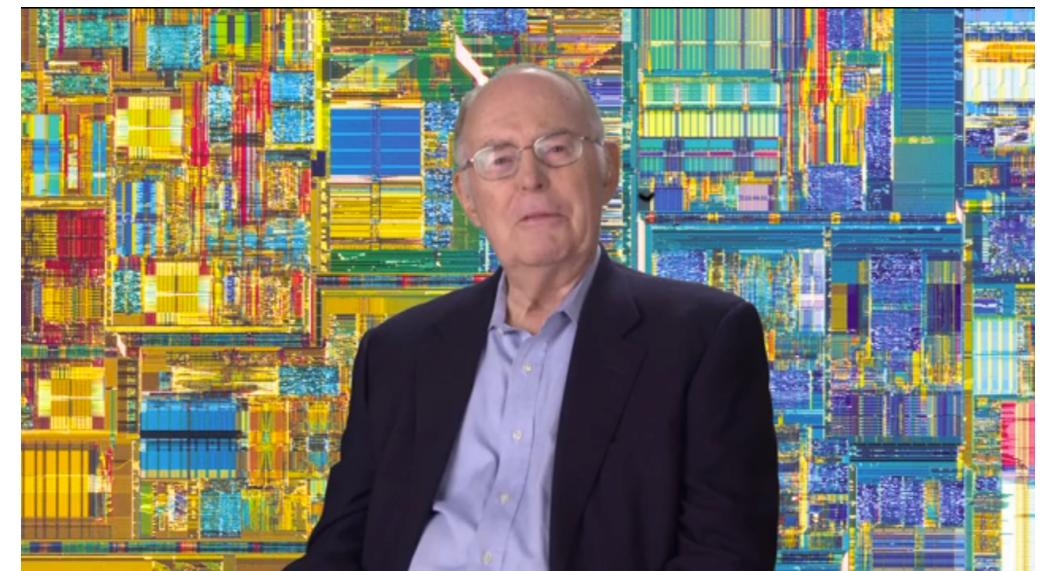
01 - Introduction

Basic Terminology

Prefix	Symbol	Size
Kilo	K	10^3
Mega	M	10^6
Giga	G	10^9
Tera	T	10^{12}
Peta	P	10^{15}
Exa	E	10^{18}
Zeta	Z	10^{21}

Moore's Law

9



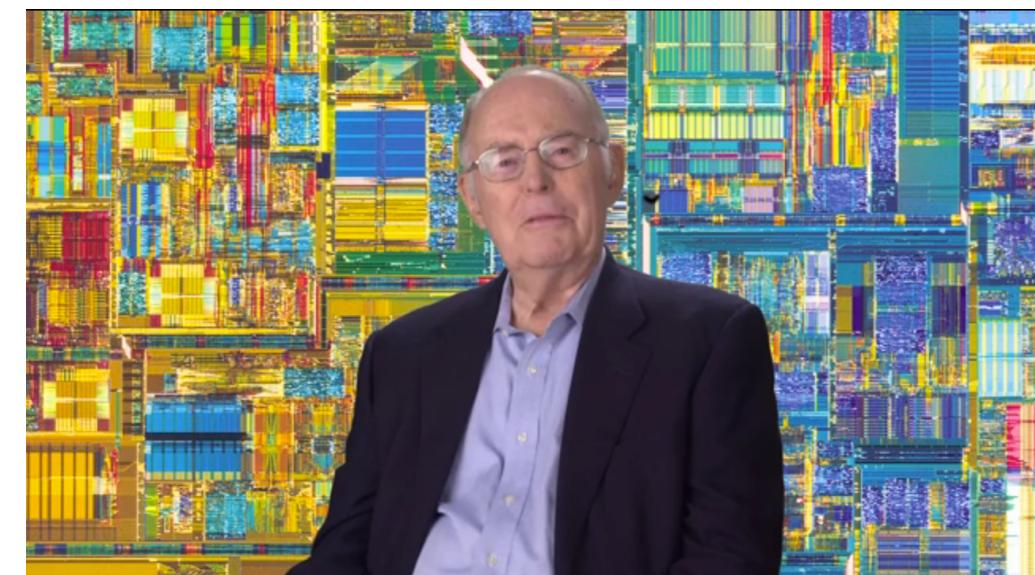
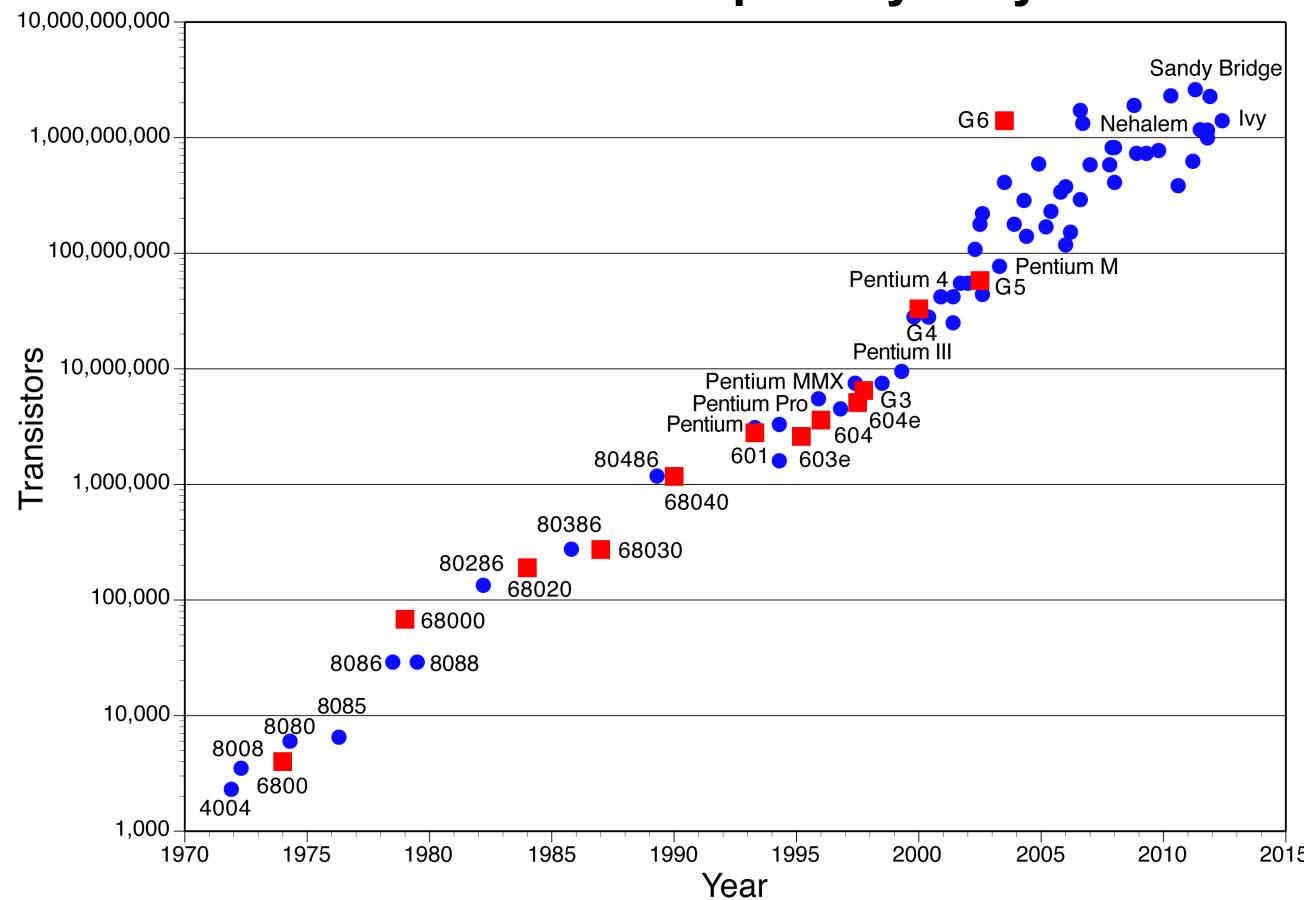
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Source: University of Wisconsin

Moore's Law

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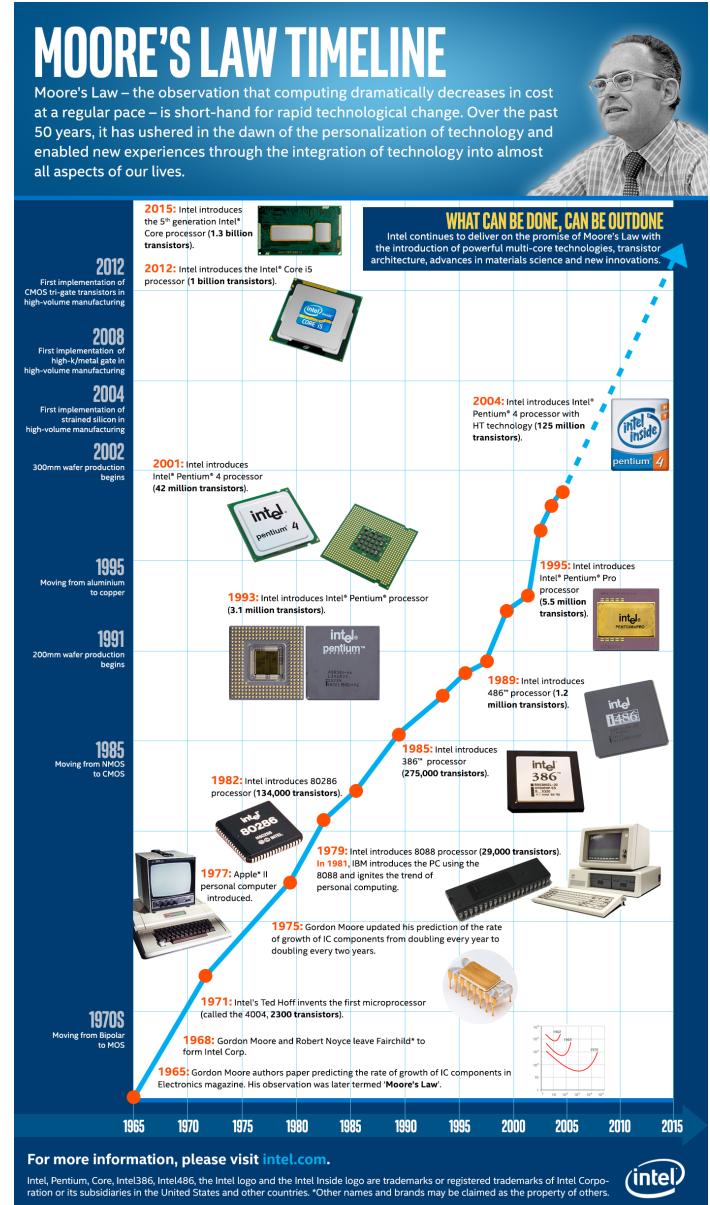
2X transistors/Chip Every 1.5 years



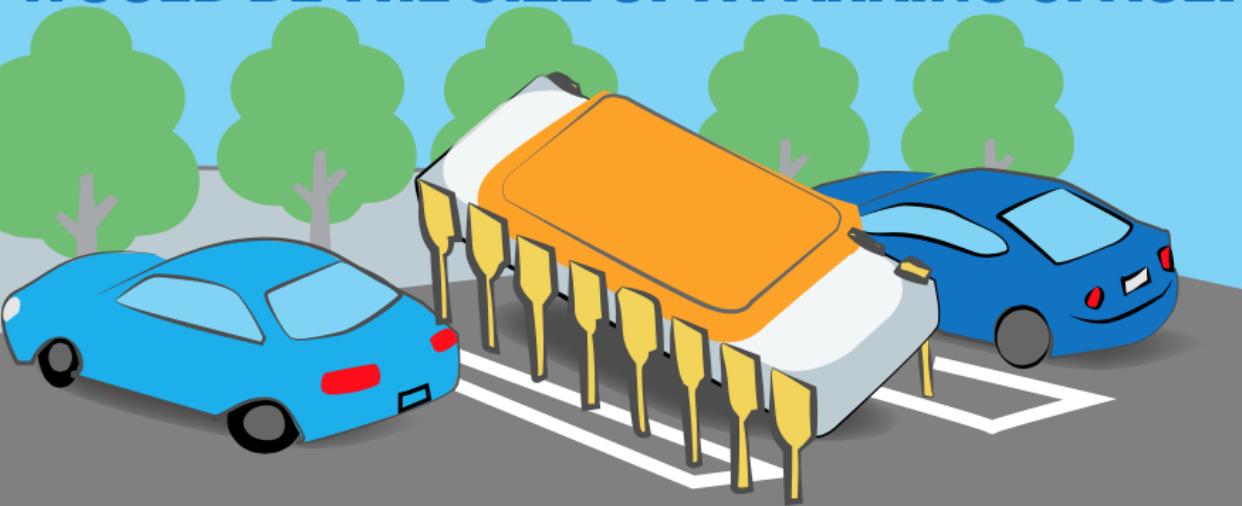
Gordon Moore (co-founder of Intel) predicted in 1965 that the transistor density of semiconductor chips would double roughly every 18 months.

In other words

10



IF AN INTEL-BASED ANDROID** PHONE WERE BUILT USING 1971 TECHNOLOGY, THE PHONE'S MICROPROCESSOR ALONE WOULD BE THE SIZE OF A PARKING SPACE.



<http://www.techspot.com/news/60418-50-years-moore-law-fun-facts-timeline-infographic.html>

How does it impact me?

11

Moore's Law: Same Chip → 2x transistors

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2. Clock rate goes up by x because wires are shorter
actually less than x , because of power consumption

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So most programs x^3 times faster, without changing them

In that case, why bother?

12

*If performance is doubling, then why bother with all this.
Just wait for computing to catch up??*

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*If performance is doubling, then why bother with all this.
Just wait for computing to catch up??*

- All major processor vendors are producing *multicore* chips
 - Every machine will soon be a parallel machine
 - To keep doubling performance, parallelism must double
- Which (commercial) applications can use this parallelism?
 - Do they have to be rewritten from scratch?
- Will all programmers have to be parallel programmers?
 - New software model needed
 - Try to hide complexity from most programmers – eventually
 - In the meantime, need to understand it

How do we measure this performance gain?

13

FLOPS – **Floating-point Operations Per Second** – The unit of measuring **RAW** computer performance

How do we measure this performance gain?

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FLOPS – Floating-point Operations Per Second – The unit of measuring **RAW** computer performance

Intel Xeon E5 2600 Sandy Bridge 2.6Ghz processor

- 8 cores
- single precision FLOPS: 16/cycle
- double precision FLOPS: 8/cycle

What is the theoretical peak performance?

How do we measure this performance gain?

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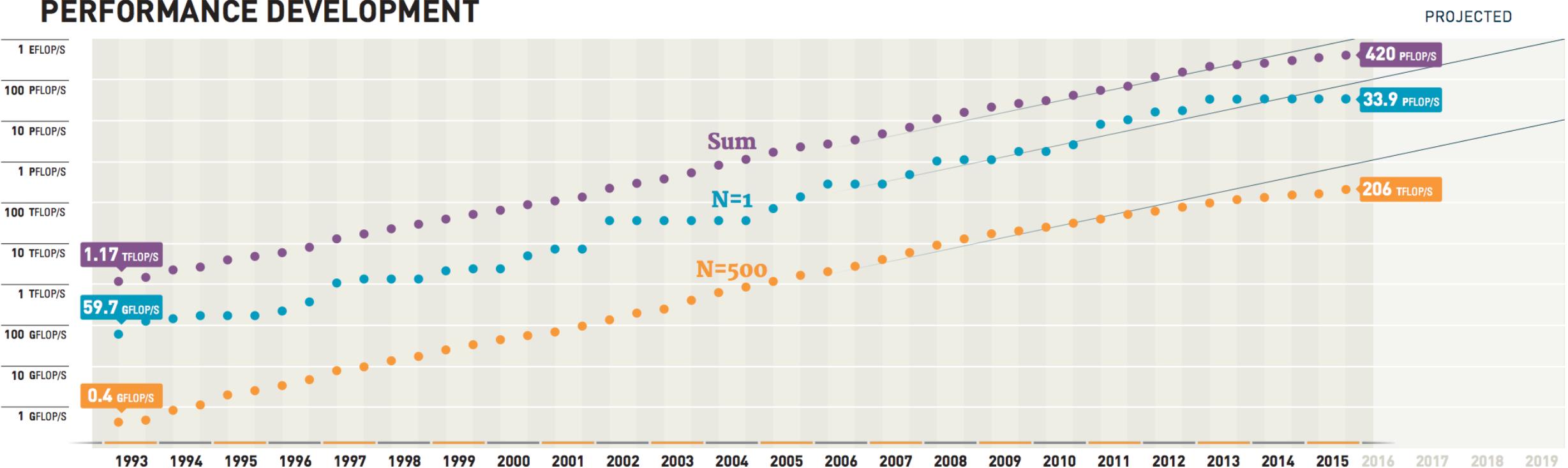
$$2.6 * 10^9 * 16 * 4 * 2$$

= 332.8Gflops (single precision)

$$2.6 * 10^9 * 8 * 4 * 2$$

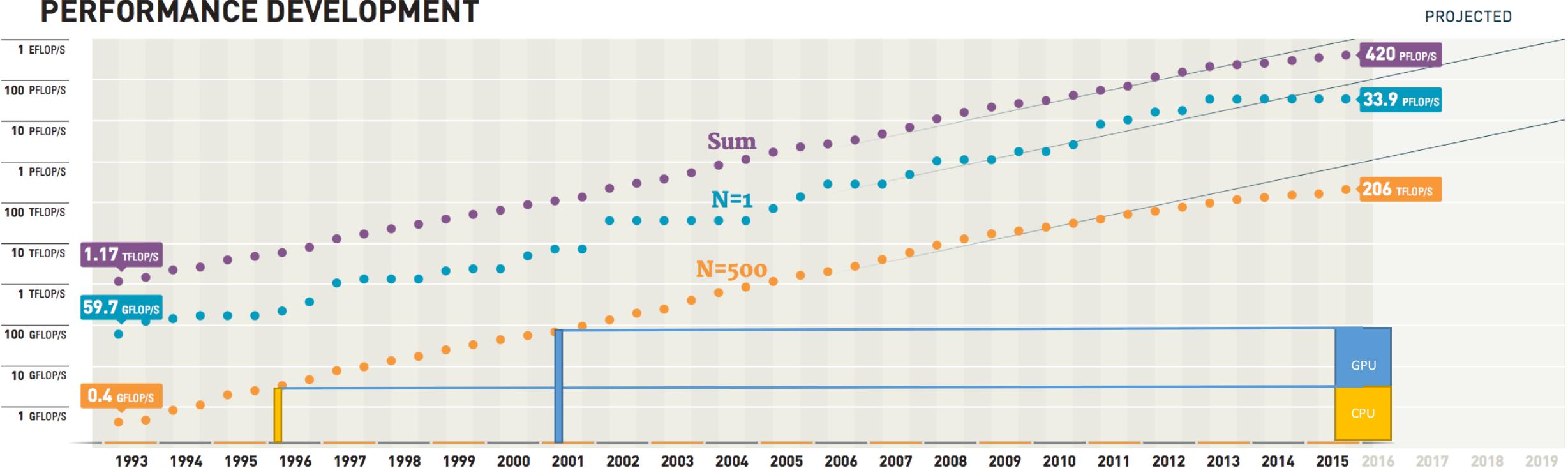
= 166.4Gflops (double precision)

PERFORMANCE DEVELOPMENT



	NAME	SPECS	SITE	COUNTRY	CORES	R _{MAX} PFLOP/S	POWER MW
1	Tianhe-2 (Milkyway-2)	Intel Ivy Bridge (12C 2.2 GHz) & Xeon Phi (57C 1.1 GHz), Custom interconnect	NUDT	China	3,120,000	33.9	17.8
2	Titan	Cray XK7, Opteron 6274 (16C 2.2 GHz) + Nvidia Kepler GPU, Custom interconnect	DOE/SC/ORNL	USA	560,640	17.6	8.2
3	Sequoia	IBM BlueGene/Q, Power BQC (16C 1.60 GHz), Custom interconnect	DOE/NNSA/LLNL	USA	1,572,864	17.2	7.9
4	K computer	Fujitsu SPARC64 VIIIfx (8C 2.0 GHz), Custom interconnect	RIKEN AICS	Japan	705,024	10.5	12.7
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What is HPC?

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High Performance Computing most generally refers to the practice of aggregating computing power in a way that delivers much higher performance than one could get out of a typical desktop computer or workstation in order to solve large problems in science, engineering, or business – InsideHPC

Tools to help do large scale, compute and/or data intensive problems

What is HPC...

16

- CPU Intensive → Distributed Memory (GPU, OpenMP) vs. Shared Memory (MPI)
- CPU Intensive vs. Data Intensive

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- CPU Intensive vs. Data Intensive
 - Data interchange vs. exploit data locality
MPI.... Hadoop...

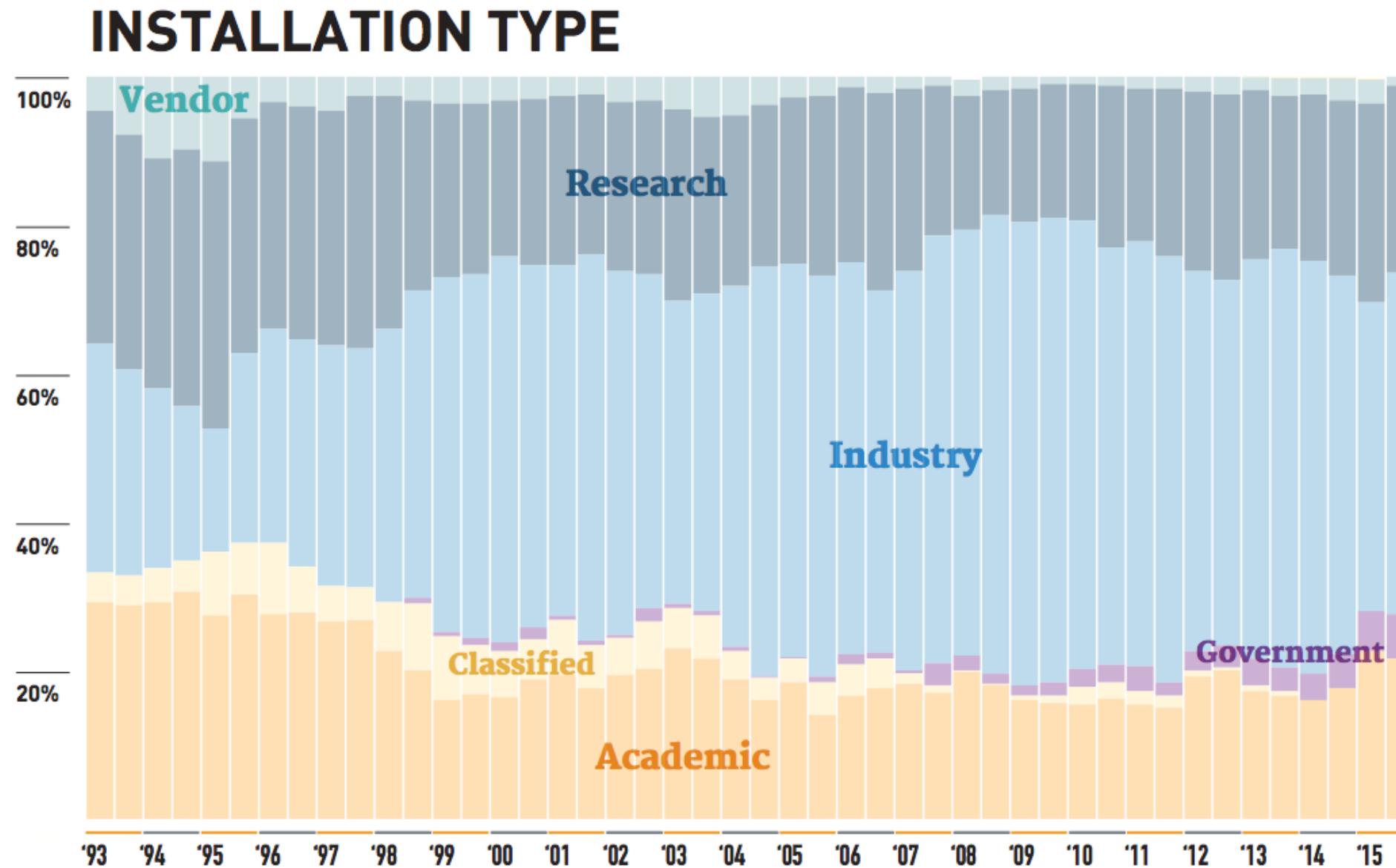
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MPI.... Hadoop...
- Architecture: CPU / GPU / Hybrid / coProcessors

Who uses HPC?

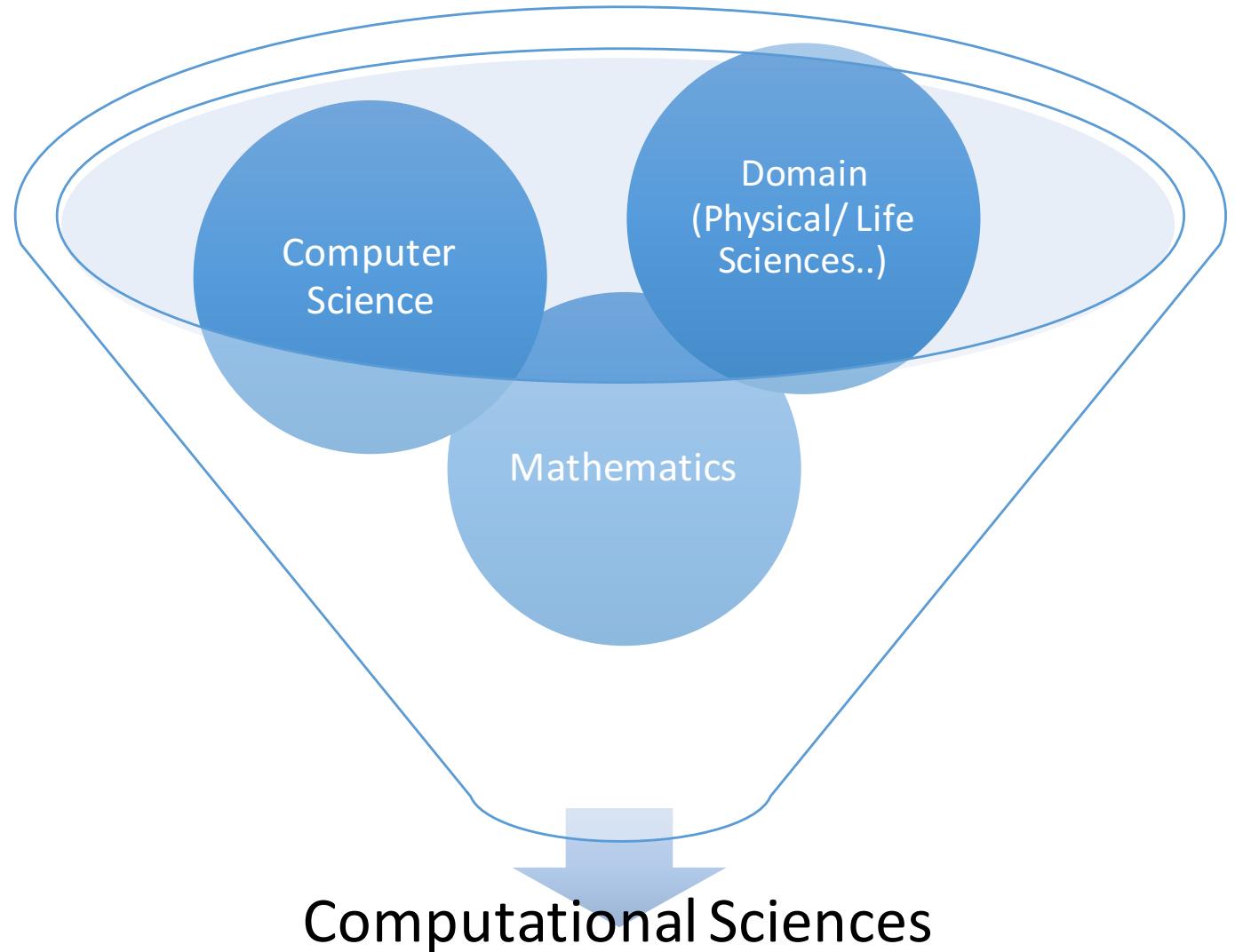
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Where is HPC used?

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- Bioinformatics and Computational Biology
- Biomedical Informatics
- Cancer Research
- Computer Vision
- Drug Discovery
- Game Shows (IBM Watson)
- Material Sciences
- Movies
- Natural Language Processing
- Nuclear Fusion
- Precision Medicine
- Retail
- Weather modeling and Prediction



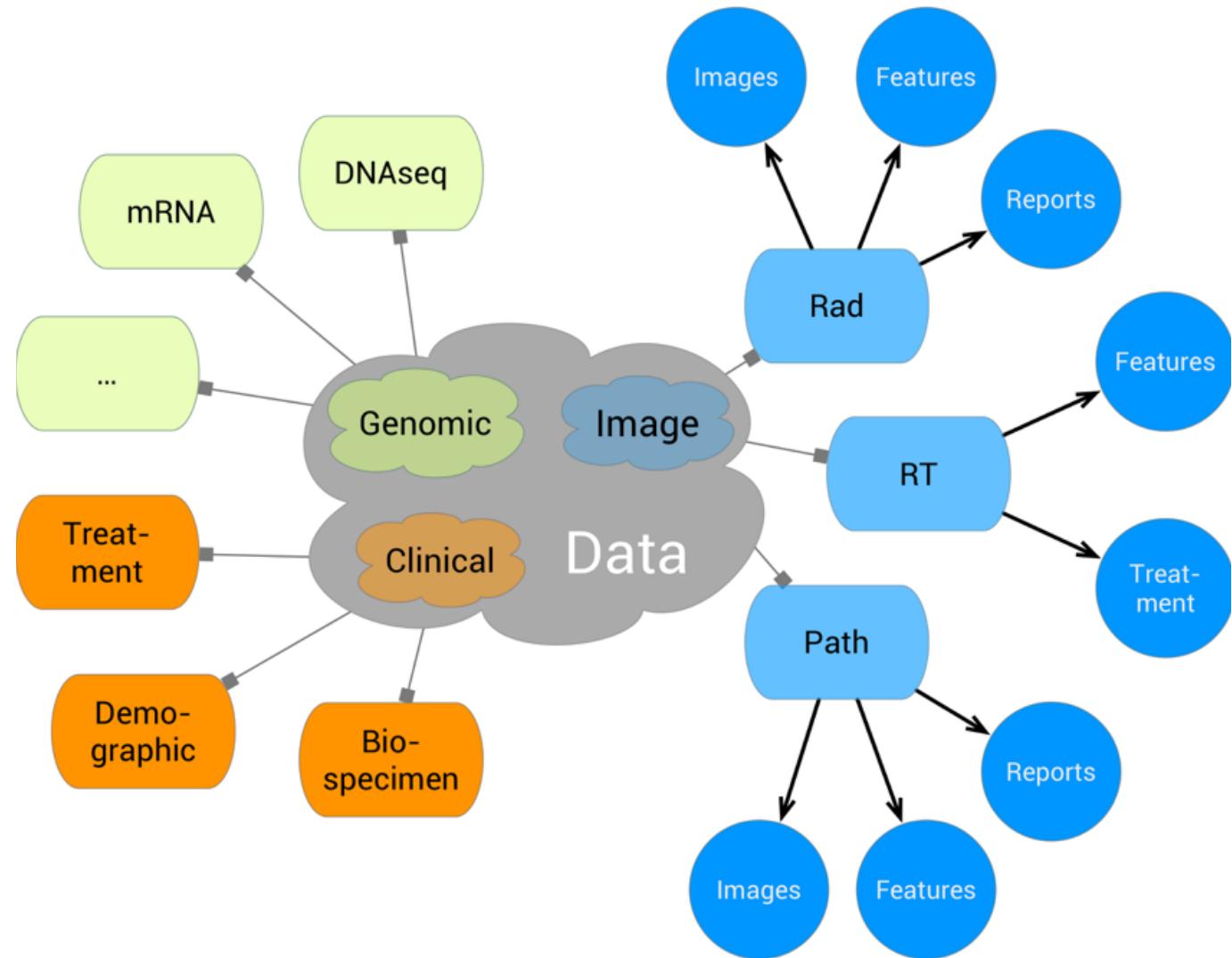
DATA CHARACTERISTICS

Large number of small datasets
Structured...Semi-structured ...

Unstructured...Ill formed
Noisy and Fuzzy/Uncertain
Spatial, Temporal relationships

DATA MANAGEMENT

Variety in storage and messaging protocols
No shared interface

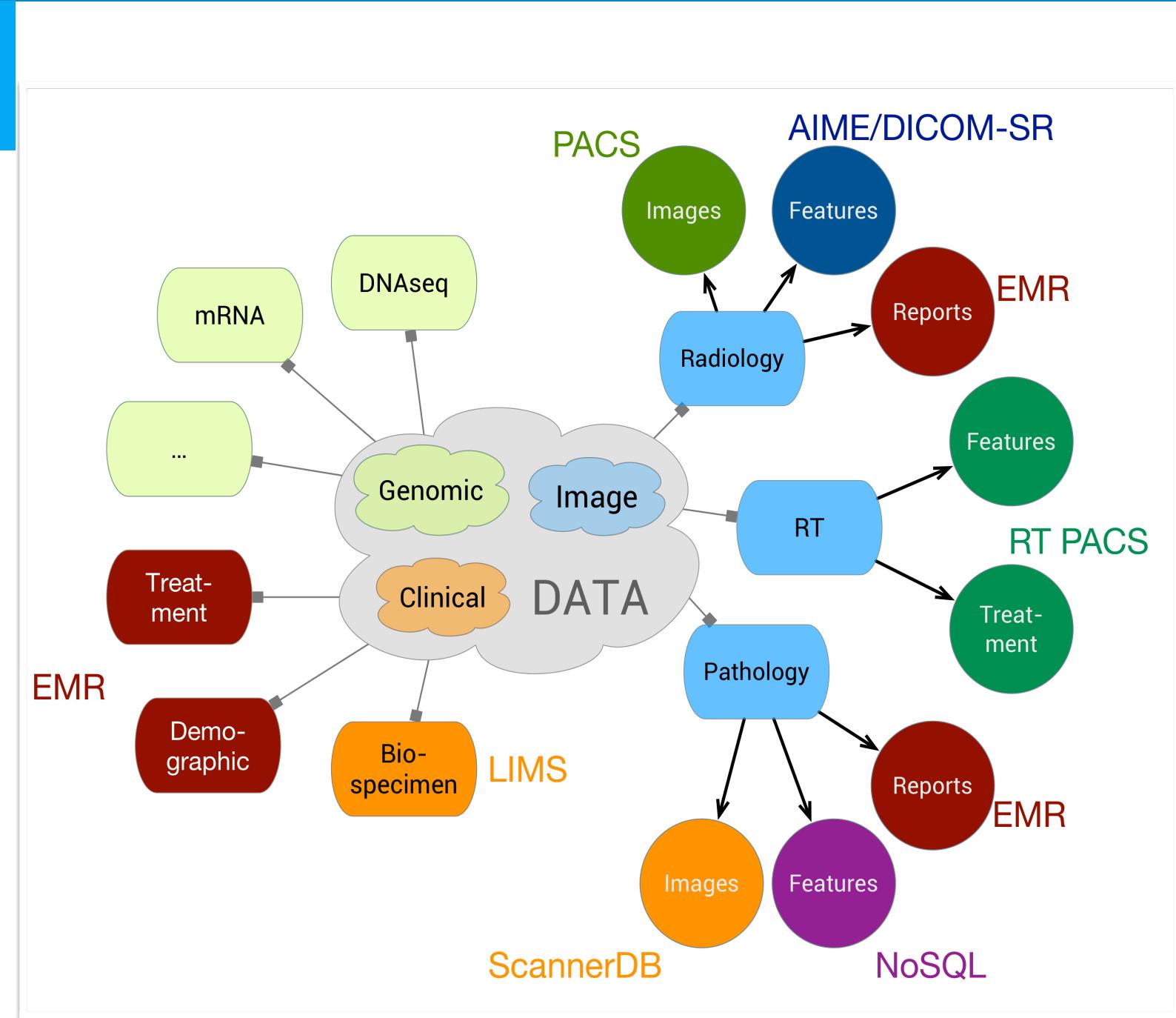


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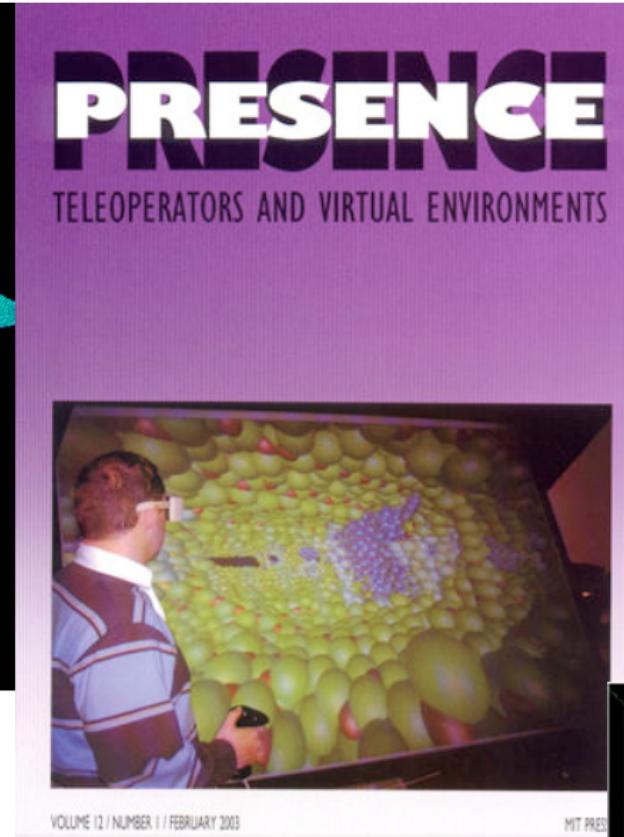
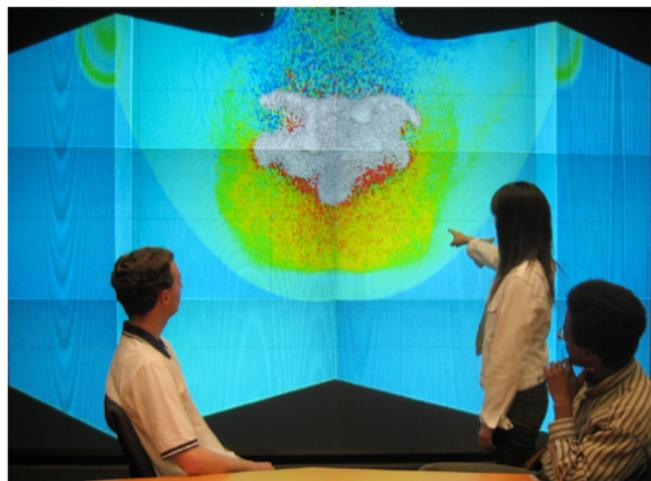
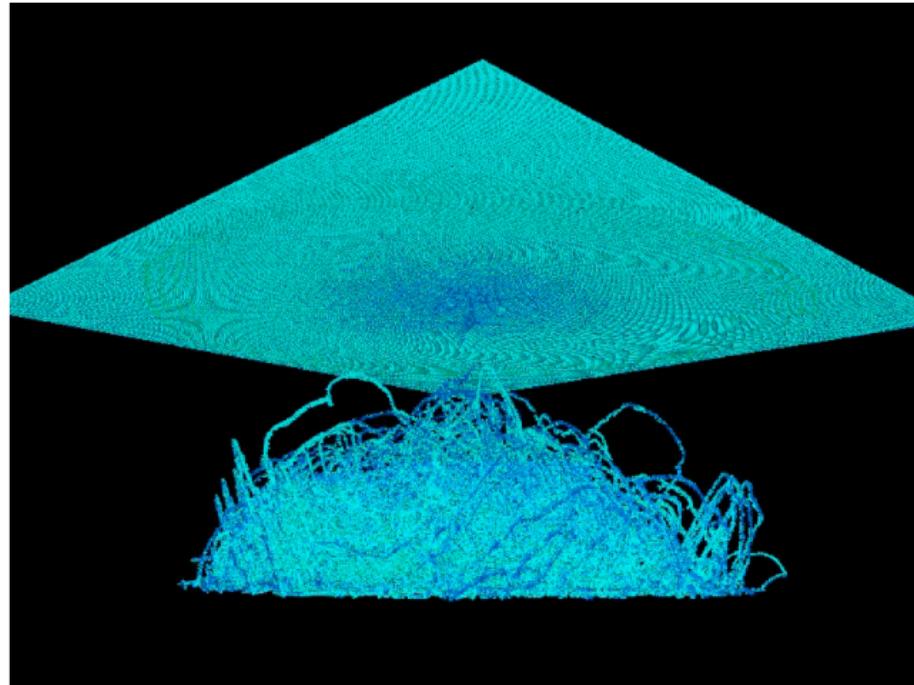
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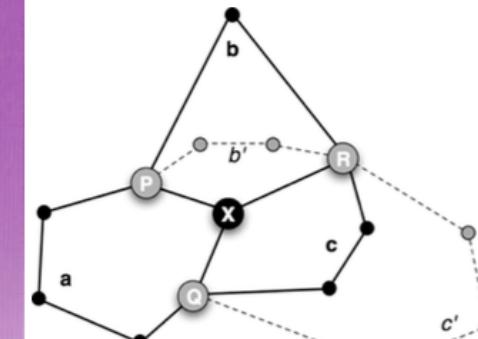


Material Science

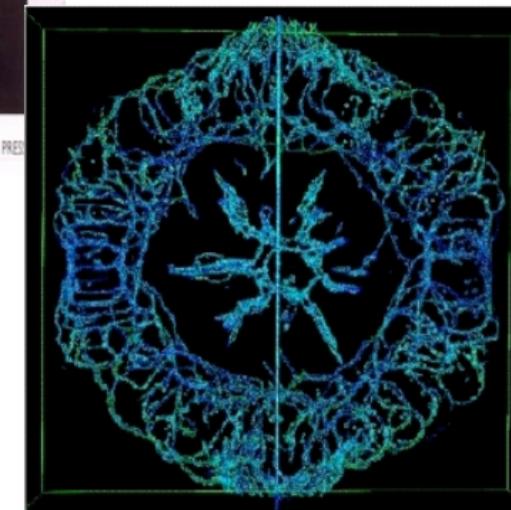
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**Immersive & interactive
visualization of
billion atoms**



**Graph-based
data mining of
chemical bond
network topology**



Hollywood



- DreamWorks has a "render farm" of servers made up of about 20,000 processors (HP BladeSystem c-Class server blades).
- The image rendering jobs are broken up into small pieces, distributed out to the server farm, and are later recompiled to create the final images for a film.
- Required a whopping 80 million compute hours to render, 15 million more hours than DreamWorks' last record holder, "The Rise of the Guardians."
- Between 300 and 400 animators worked on "The Croods" over three years.
- After completing a film, about 70TB worth of data (things like background art or plants) is stored for future usage in future productions.

Course Outline (Tentative)

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Hardware, programming methodologies and algorithms for high performance and **large-scale** computing

Theme	Specific Topics
Introduction	Overview of The Course Incl. Prerequisites; HPC In The Age of Big Data; Architectural And Networking Advances; Parallel And Distributed Programming Models
HPC Hardware and Systems	Parallel Architectures; Networking; High Speed Interconnects; GPUs; Measuring Performance and Scalability; Storage Systems; Containers
Parallel Computing Frameworks	Designing algorithms for parallelism; Problem/Data Partitioning; Optimization Techniques; Load Decomposition;
Traditional Parallel Programming Models	Programming with OpenMP; Programming with MPI
Distributed/Cloud Computing	Cloud Computing environments (IaaS, PaaS); Hadoop; Apache Spark
Applications of HPC	Material Genome, Retail, Genomics and Bioinformatics, Medical Imaging, Clinical Informatics

Learning Objectives (aka what will be covered)

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- Understand what is HPC – strengths and limitations
- Hardware and Programming Methodologies
- Develop an intuition for CPU-intensive vs. data-intensive computing
- Learn from the experiences of others
- Learn through hands-on problems and projects

What is not covered in this course

24

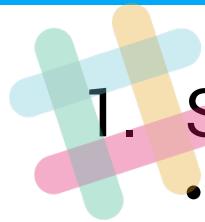
- GPUs, CUDA...
- Machine learning algortihms
- Deep dive into parallel processing algortihms
- Optimization techniques

Assignment #1

Due: 11:59pm, 01/17/2016

Assignment #1 (Due 01/17/2016)

26



1. Signup on class team: hpccourse.slack.com
 - Introduce yourself on the #general channel
2. Two programming assignments to help me establish a baseline
 - No help from instructor on this one
 - No help from fellow students on any aspect of this assignment

Assignment #1 (Due 01/17/2016)

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Submission:

1. Create a **private** github repo: name-hpc2016
 - <https://education.github.com>
2. Add me as a collaborator to the repo (sharmaashish)
3. Create folders per assignment: HW1/HW2...
 - Case sensitive
4. Commit your assignment to the appropriate folder
5. I will checkout your latest commit made on or before the due date
 - Always include a brief README.md with instructions on how to test your code

Assignment #1 (Due 01/17/2016)

28

- Matrix Multiplication
 - Create a random $n \times n$ matrix A
 - Multiply A x A
 - Give user the ability to specify the size of the matrix as an input parameter (-n 3)
 - Give user the option to display the input and product (-display)
 - Display how long it takes to run this on a 2x2, 4x4, 8x8, 16x16...4096x4096 (-benchmark)
- Submission:
 1. Profile your submission to determine what parts take up the most amount of time. Are there parts of your code that are impacted by the size of n? Any optimization strategies?
 2. Submit C/C++/Python code w/ makefile (C/C++) → make and/or run.sh

sh run.sh -n 3 -display

sh run.sh -benchmark

Assignment #1 (Due 01/17/2016)

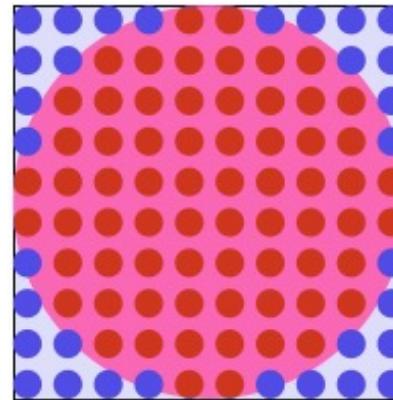
29

- Calculate the value of π

Throw n random points on a square

Count those points that land in a circle

$$\text{PI} = 4 * \text{num of points in the circle} / \text{num of points}$$



- Submission:

1. Profile your submission to determine what parts take up the most amount of time. Are there parts of your code that are impacted by the size of n ? What is the % error between your PI and π ? Any optimization strategies?
2. Submit C/C++/Python code w/ makefile (C/C++) → make and or/run.sh

```
sh run.sh -n 10000
```



HPC Hardware

HPC Programming Paradigms

HPC Algorithms

Distributed/Cloud Computing and HPC

IaaS, PaaS and SaaS

Data Management