

# High-Performance Computing (HPC)

## **Understanding the Power of Supercomputers**

**An Introduction for Beginners**

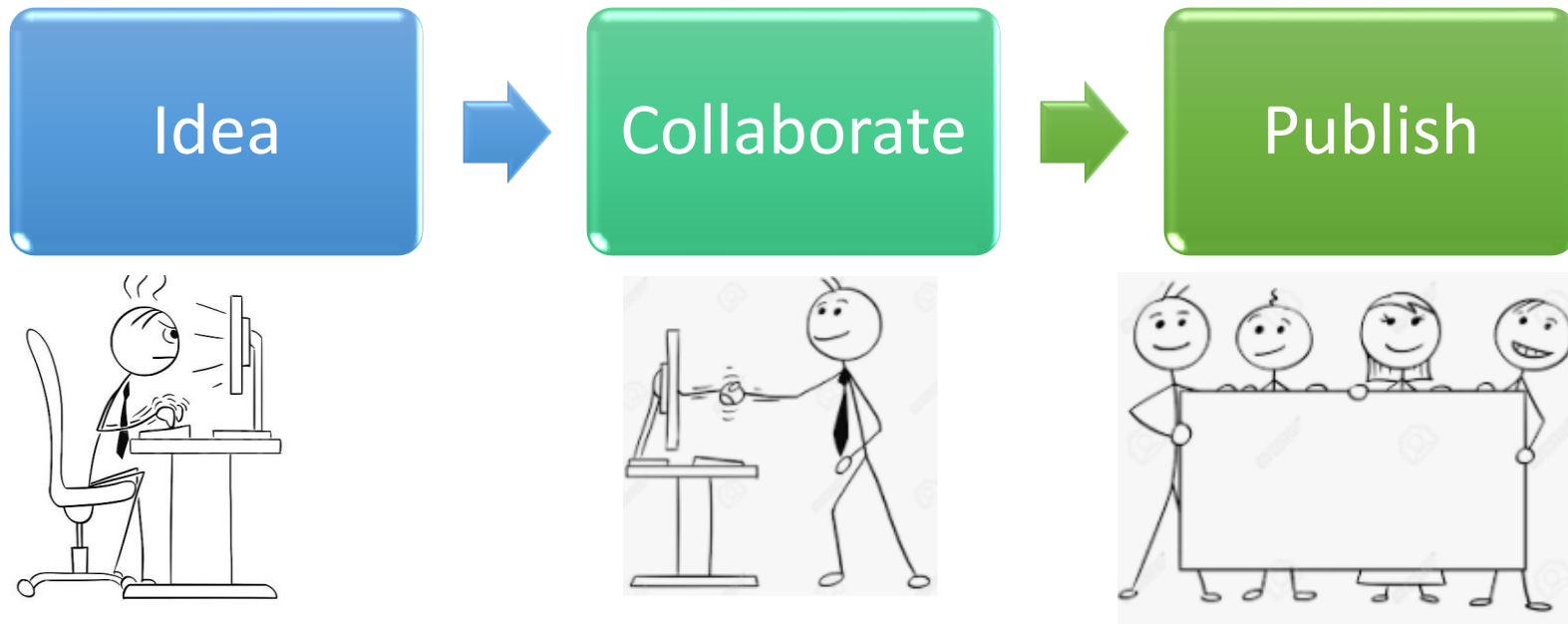
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Researcher at eScience/Supercomputing/IT

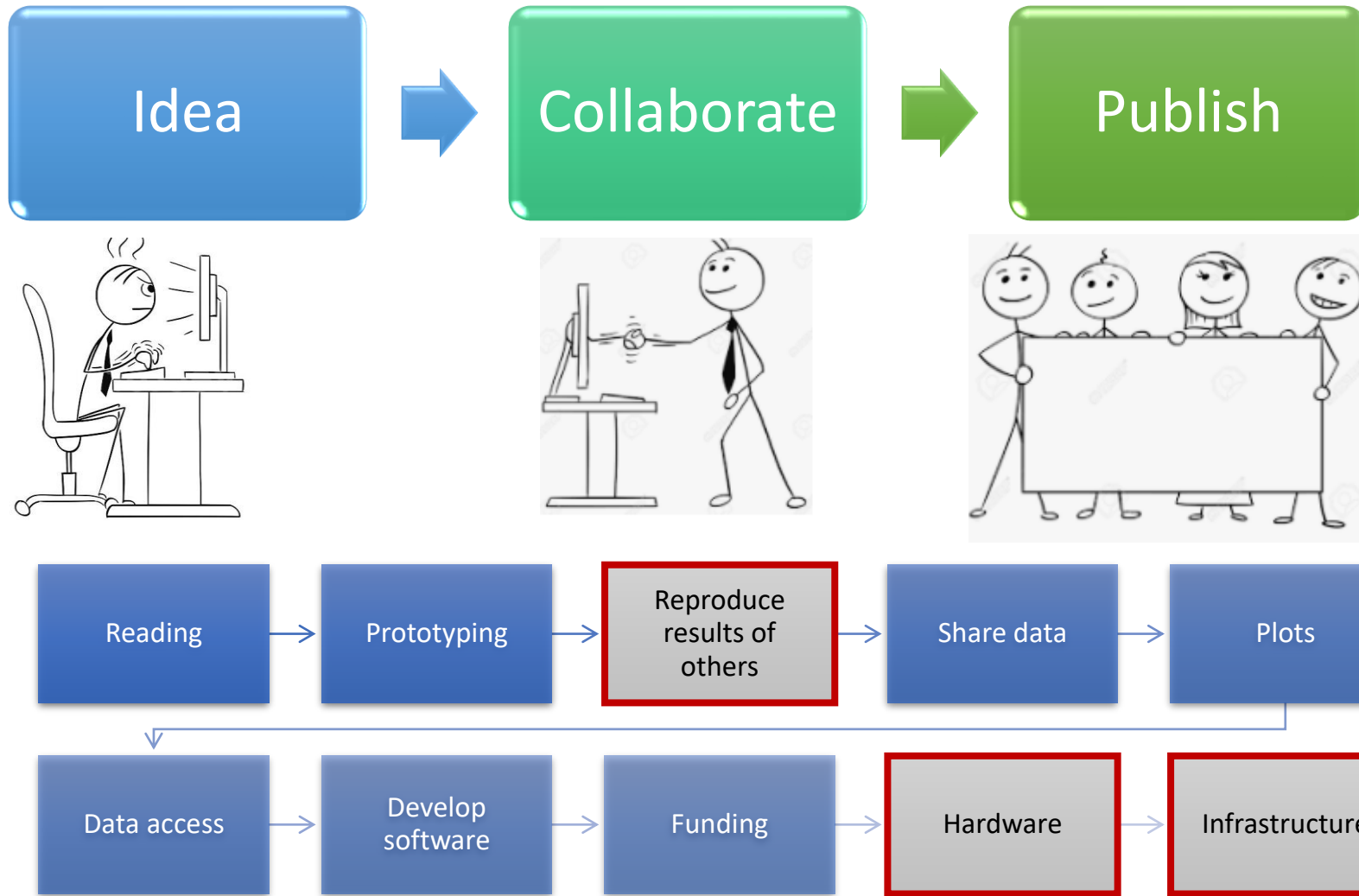
Leibniz-Institut für Astrophysik Potsdam (AIP), Germany

AIP,2025

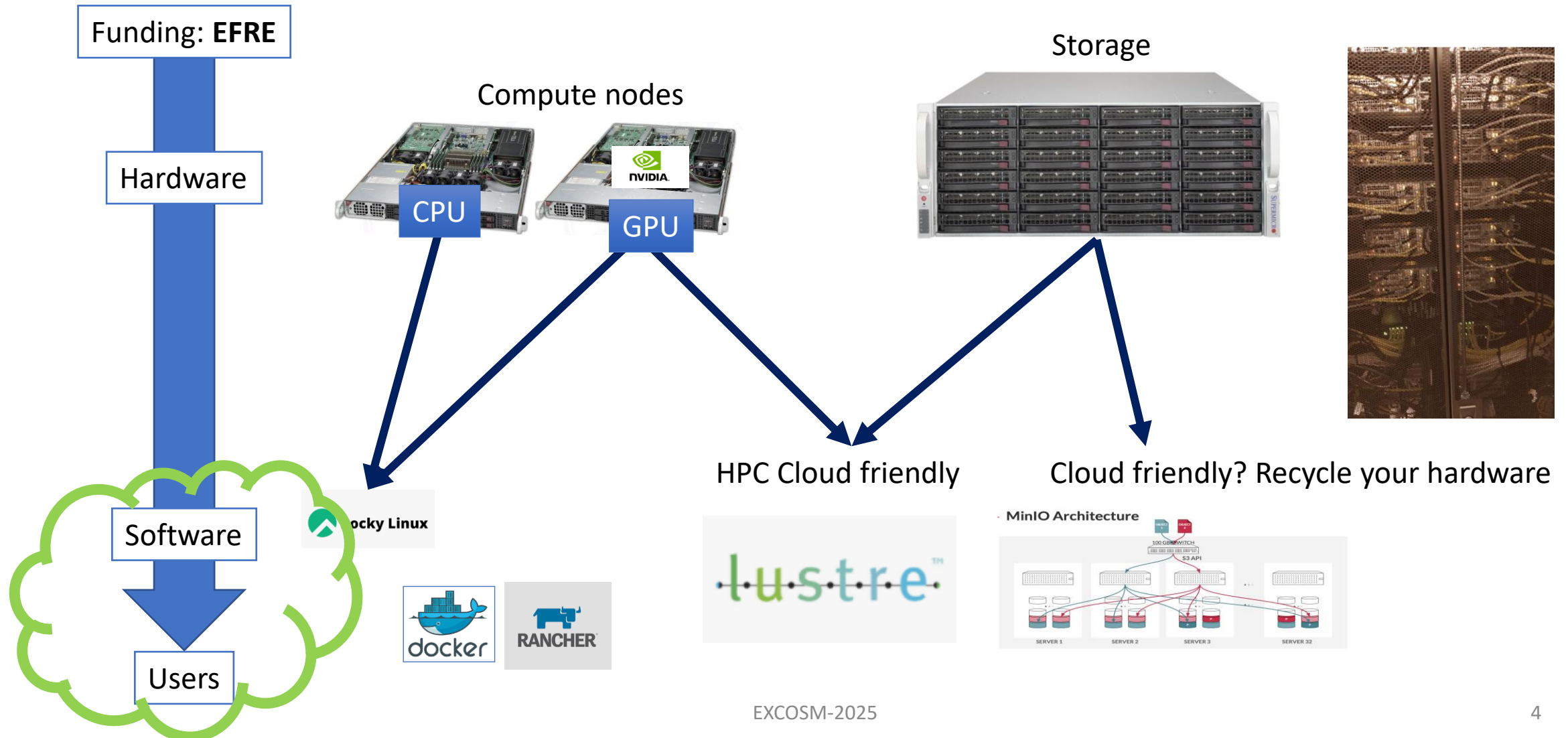
# Scientific life (top to down)



# Scientific life (top to down)



# Infrastructure (down to top)



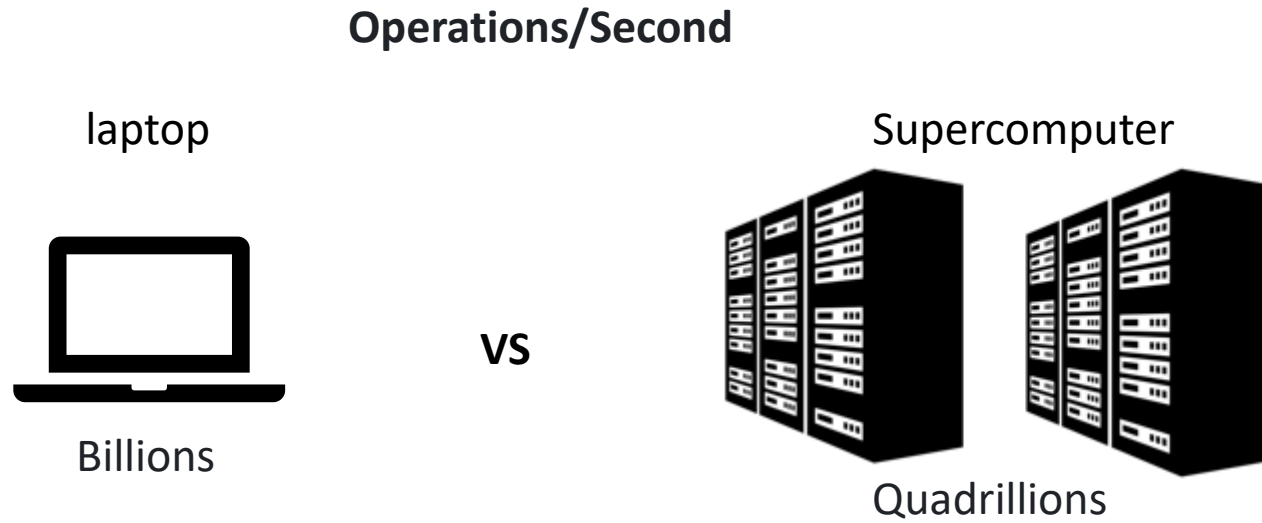
# What is High-Performance Computing (HPC)?

- HPC combines computing power to deliver higher performance
- Multiple computers working together as one system
- Solves complex problems faster than regular computers
- Think of it as a "*supercomputer*"

# What is High-Performance Computing (HPC)?

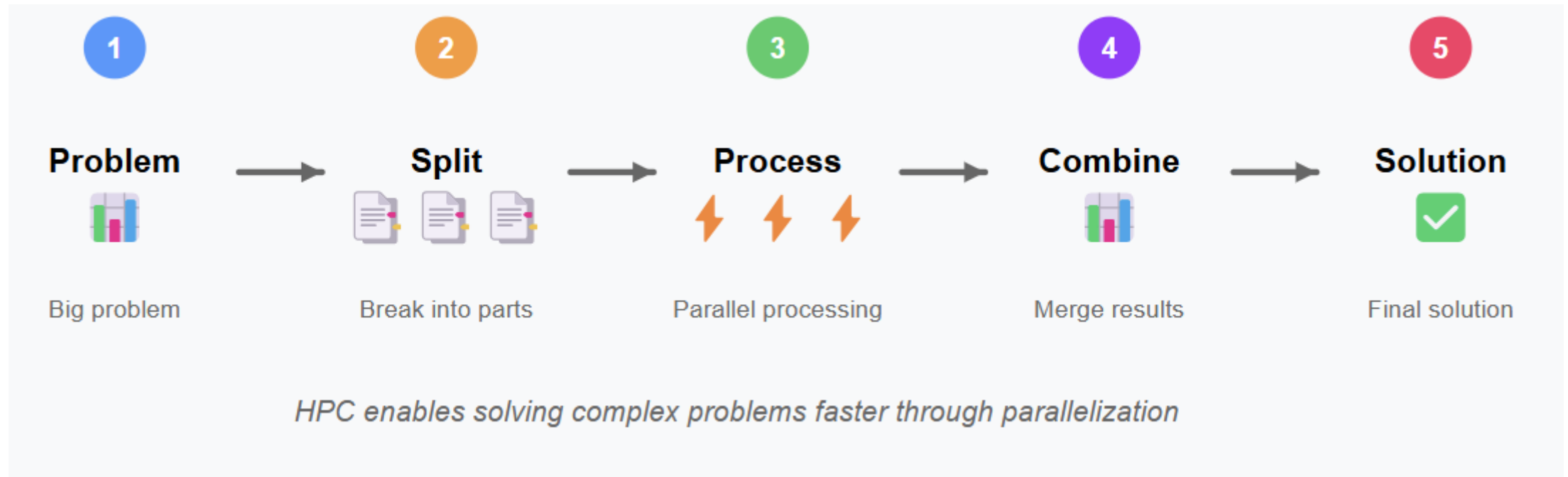
- **Definition:** Computing systems with capabilities significantly beyond typical desktop computers
- **Key characteristics:**
  - Massive parallelization
  - High-speed interconnects
  - Specialized hardware
  - Advanced cooling systems
  - Custom software environments
- **Scale:** From small clusters to the world's fastest supercomputers

# The Scale of HPC



*1 Quadrillion = 1,000,000,000,000,000*

# How Does HPC Work?

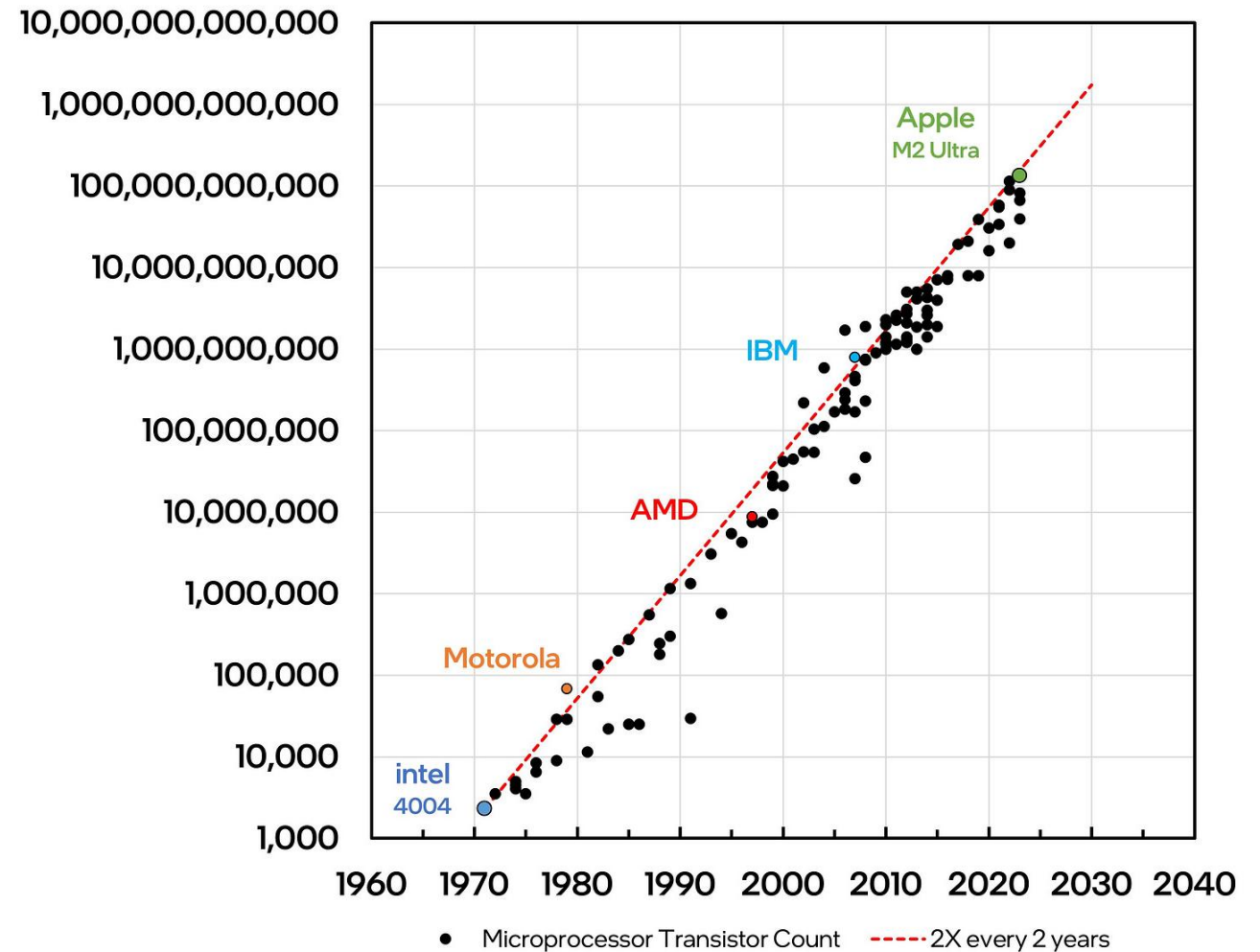




# The Evolution of HPC

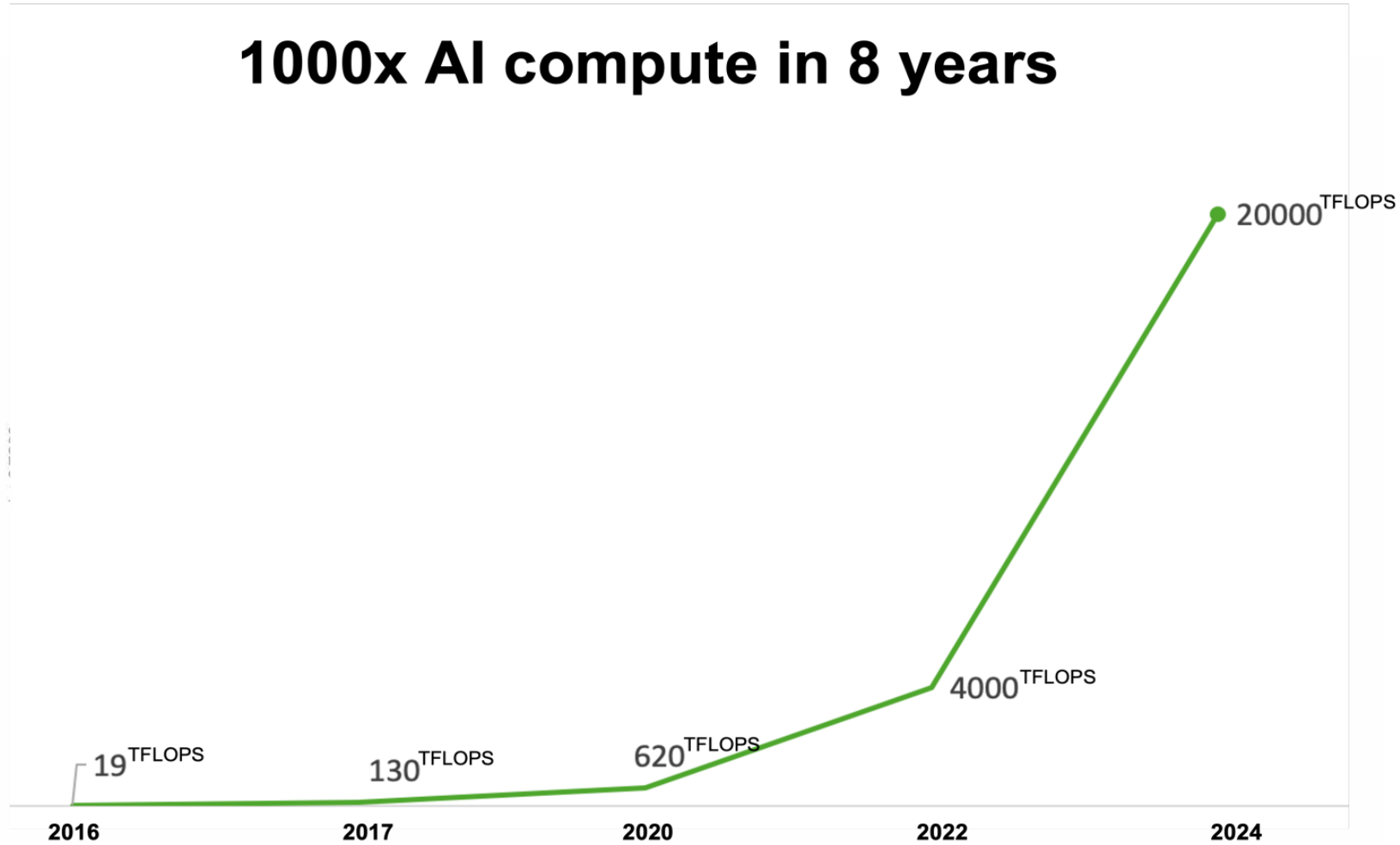
- 1960s**: First supercomputers (CDC 6600, IBM 7030)
- 1980s**: Vector processing (Cray-1, Cray-2)
- 1990s**: Massive parallel processing
- 2000s**: Cluster computing
- 2010s**: Heterogeneous computing (CPU + GPU/FPGA)
- 2020s**: Exascale computing and specialized AI systems

## Exponential growth of CPU-based computing power



Moore's law is the observation that the number of transistors in an integrated circuit (IC) doubles about every two years.

# But GPUs are following Huang's Law



He observed that Nvidia's GPUs were "25 times faster than five years ago"!

# Components of an HPC System

- **Compute Nodes:** Thousands of processors working together
- **Network:** High-speed, low-latency interconnects (InfiniBand, OmniPath), 100+ Gb/s, <1 microsecond
- **Storage Systems:** Parallel file systems handling petabytes of data
- **Operating System:** Specialized Linux distributions
- **Job Scheduler:** Software that manages computing resources
- **Power & Cooling:** Advanced infrastructure to maintain operation

# HPC Architecture Basics

## Key Architectural Models:

- **Shared Memory:** Multiple processors accessing the same memory space
- **Distributed Memory:** Each processor has its own memory
- **Hybrid Systems:** Combination of shared and distributed memory
- **Accelerated Systems:** CPUs paired with GPUs or other accelerators

# Measuring HPC Performance

## Key Metrics:

- **FLOPS** (Floating Point Operations Per Second)
  - TeraFLOPS (trillion  $10^{12}$ )
  - PetaFLOPS (quadrillion  $10^{15}$ )
  - ExaFLOPS (quintillion  $10^{18}$ )
- **Scalability**: How performance increases with more resources
- **Efficiency**: Ratio of actual to theoretical peak performance
- **Bandwidth**: Data transfer rates between components
- **Latency**: Time delay in communication
- As of November 2024, the world's fastest supercomputer is **El Capitan at 1.742 exaFLOPS at LLNL California**

<https://top500.org/news/el-capitan-achieves-top-spot-frontier-and-aurora-follow-behind/>

# Types of HPC Systems

## 1.Clusters

1. Connected computers
2. Common in universities

## 2.Supercomputers

1. Specialized systems
2. National facilities

## 3.Cloud HPC

1. Remote access
2. Pay-as-you-go

# Benefits of Using HPC

- Faster research results
- Better scientific models
- New discoveries
- Economic advantages
- Competitive edge
- Innovation enablement

# Who Uses HPC?

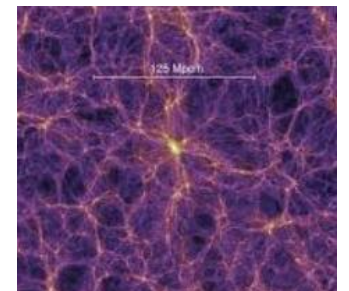
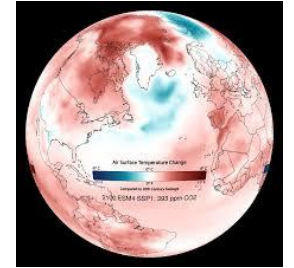
- Scientists
- Researchers
- Engineers
- Companies
- Government agencies
- Universities



# Scientific Applications

## Examples:

- **Climate Modeling:** Simulating global climate systems
  - Predicting climate change effects
  - Hurricane path prediction
- **Genomics:** DNA sequencing and analysis
  - Human Genome Project reduced from years to hours
- **Astrophysics:** Universe simulations
  - Galaxy formation models
  - Black hole collision simulations



# HPC in Astrophysics & Cosmology

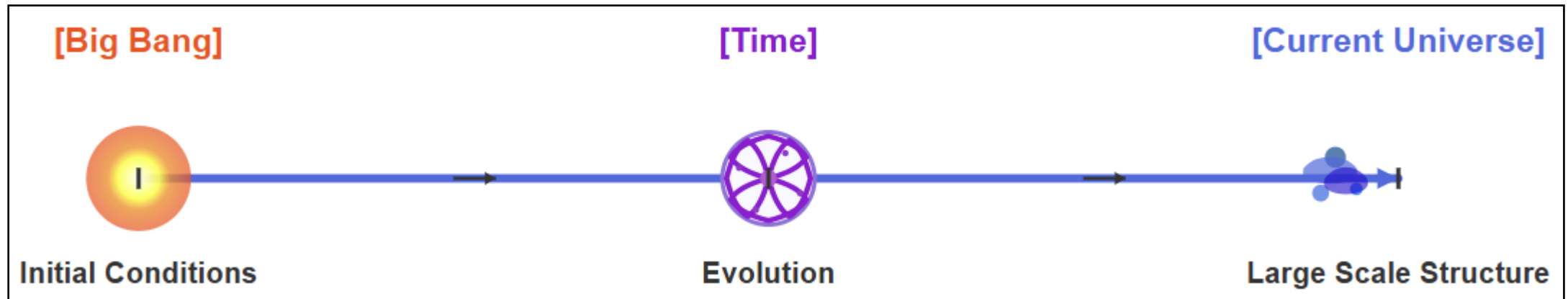
## Key Applications:

- N-body simulations
- Galaxy formation models
- Dark matter distribution
- Cosmic structure evolution
- Gravitational wave analysis

# Cosmological N-body Simulations

## What are they?

- Track motion of particles under gravity
- Model dark matter distribution
- Simulate cosmic structure formation
- Billions to trillions of particles
- Time evolution from early universe to present



# Why HPC for Cosmological Simulations?

## 1. Scale of Computation

- $10^9$  -  $10^{12}$  particles
- Long-range gravitational forces
- Multiple time steps

## 2. Memory Requirements

- Particle positions & velocities
- Force calculations
- Tree structures for optimization

## 3. Data Output

- Terabytes to Petabytes

# Famous Cosmological Simulations

## Millennium Simulation

- 10 billion particles
- 2.2 billion light-years box
- Dark matter evolution

## IllustrisTNG

- Galaxy formation physics
- Magnetic fields
- Gas dynamics
- Dark matter + baryons
- Black holes and more..

# N-body Algorithms & HPC Implementation

## Methods:

### Particle-Particle (PP)

- Direct force calculation
- $O(N^2)$  complexity

### Particle-Mesh (PM)

- Grid-based approach
- Faster but lower resolution

### Tree Codes

- Hierarchical force calculation
- Barnes-Hut algorithm

# N-body Algorithms & HPC Implementation

## Parallelization:

- Domain decomposition
- Load balancing
- MPI + OpenMP hybrid approach

# Future of HPC

- AI and machine learning
- Increased accessibility
- Green computing
- Exascale systems becoming common
- Quantum computing integration



# Getting Started with HPC

- Learn parallel programming
- Understand basic concepts
- Start with small projects
- Use university resources
- Join HPC communities

# Conclusion

- HPC is essential for modern research
- Enables solutions to complex problems
- Drives innovation and discovery
- Future of computing technology
- Growing field with many opportunities

# Questions?