

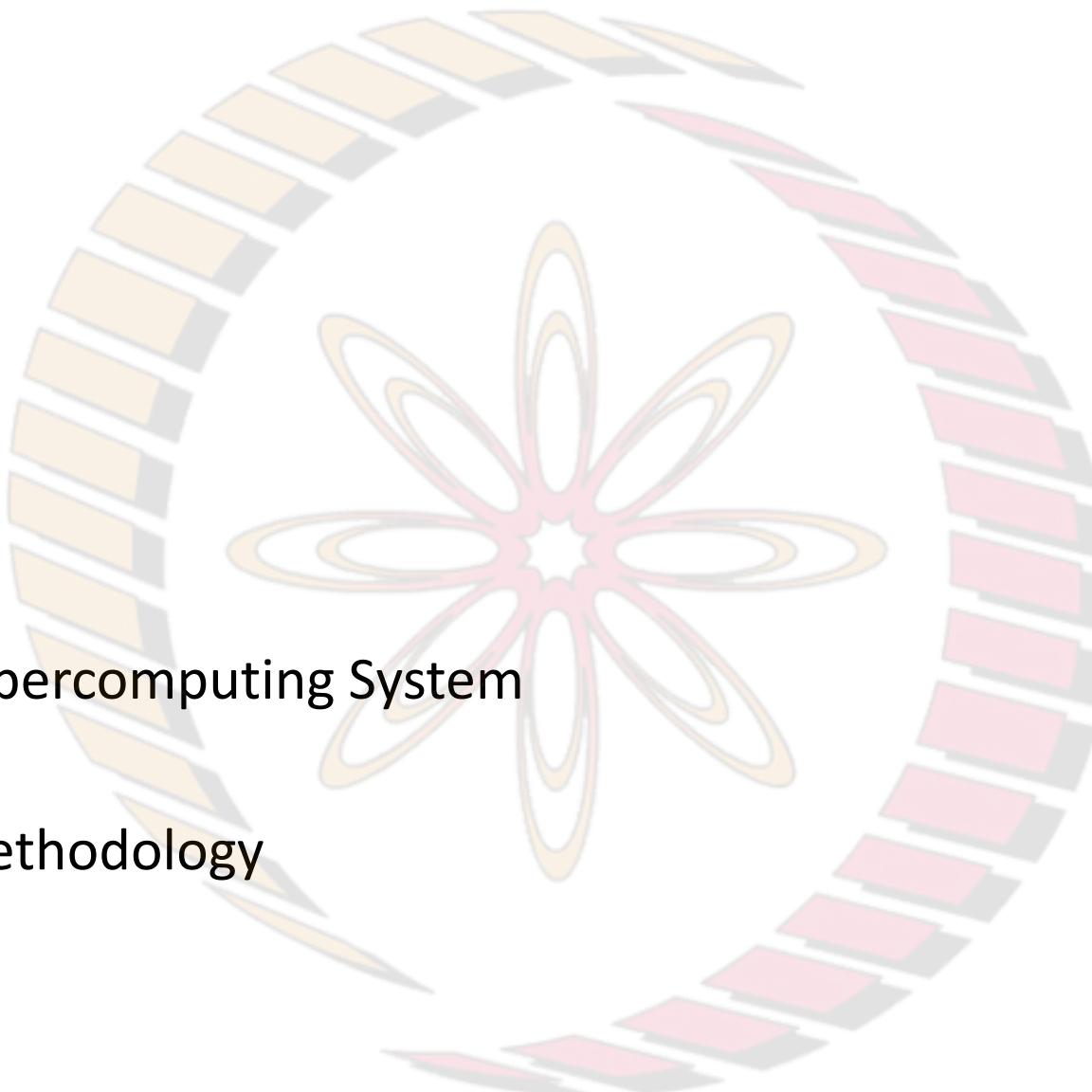


An Introduction to High Performance Computing

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Agenda

- Introduction
- Need for HPC
- Architecting a Supercomputing System
- Parallelization Methodology
- Summary



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Introduction

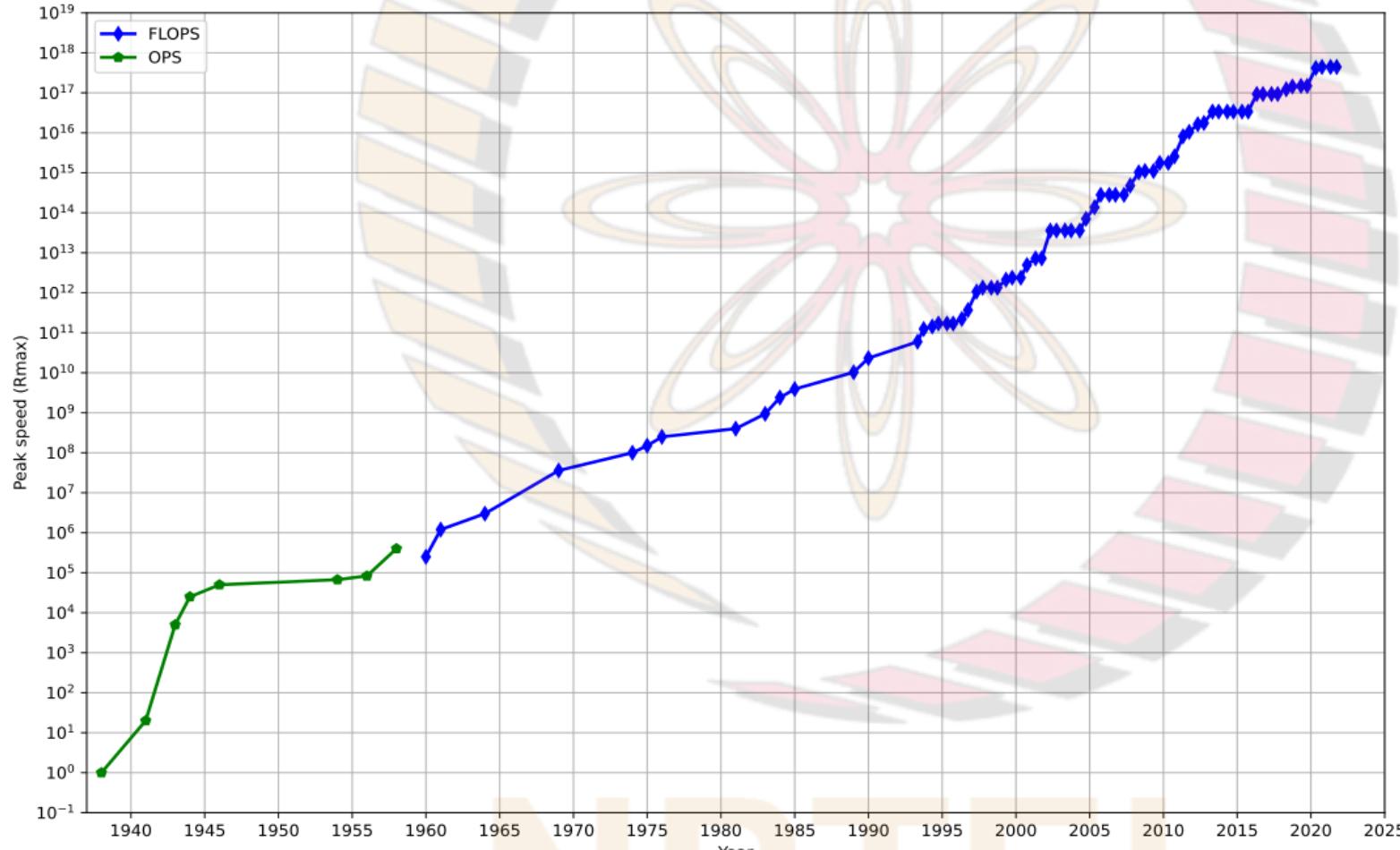
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ENIAC – Circa 1947



Image Source: Wikipedia

Top Computer Speeds over years



Source: Wikipedia

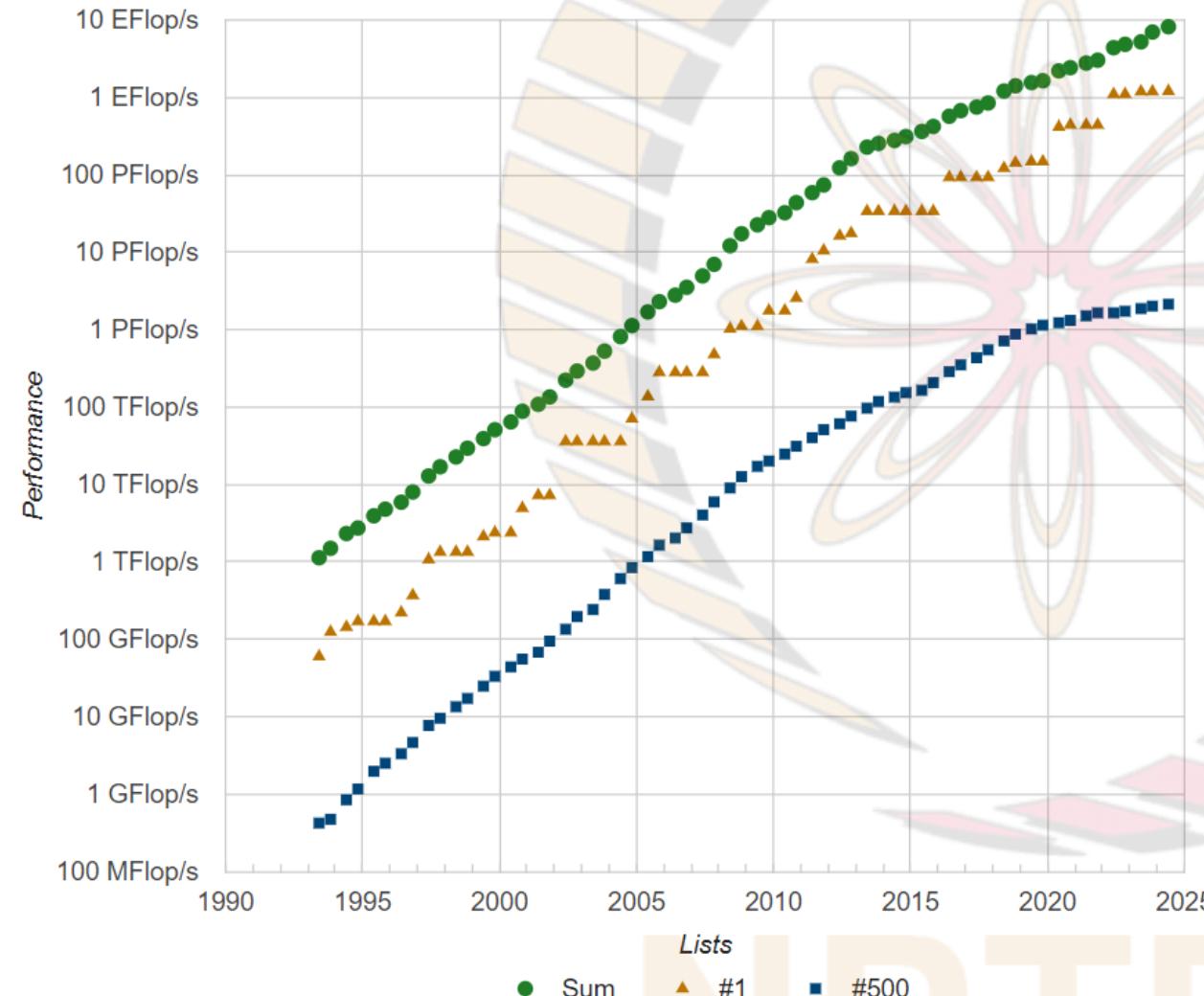
Measuring Power of Supercomputers

- Performance of supercomputers is measured using Floating point operations that it can perform in one second
 - Represented by FLOPS, flops or flop/s

Name	Represented as	Value
teraFLOPS	TFLOPS	10^{12}
petaFLOPS	PFLOPS	10^{15}
exaFLOPS	EFLOPS	10^{18}
zettaFLOPS	ZFLOPS	10^{21}
yottaFLOPS	YFLOPS	10^{24}

- Top500 website (www.top500.org) lists world's top supercomputers using a program called High Performance Linpack (HPL)

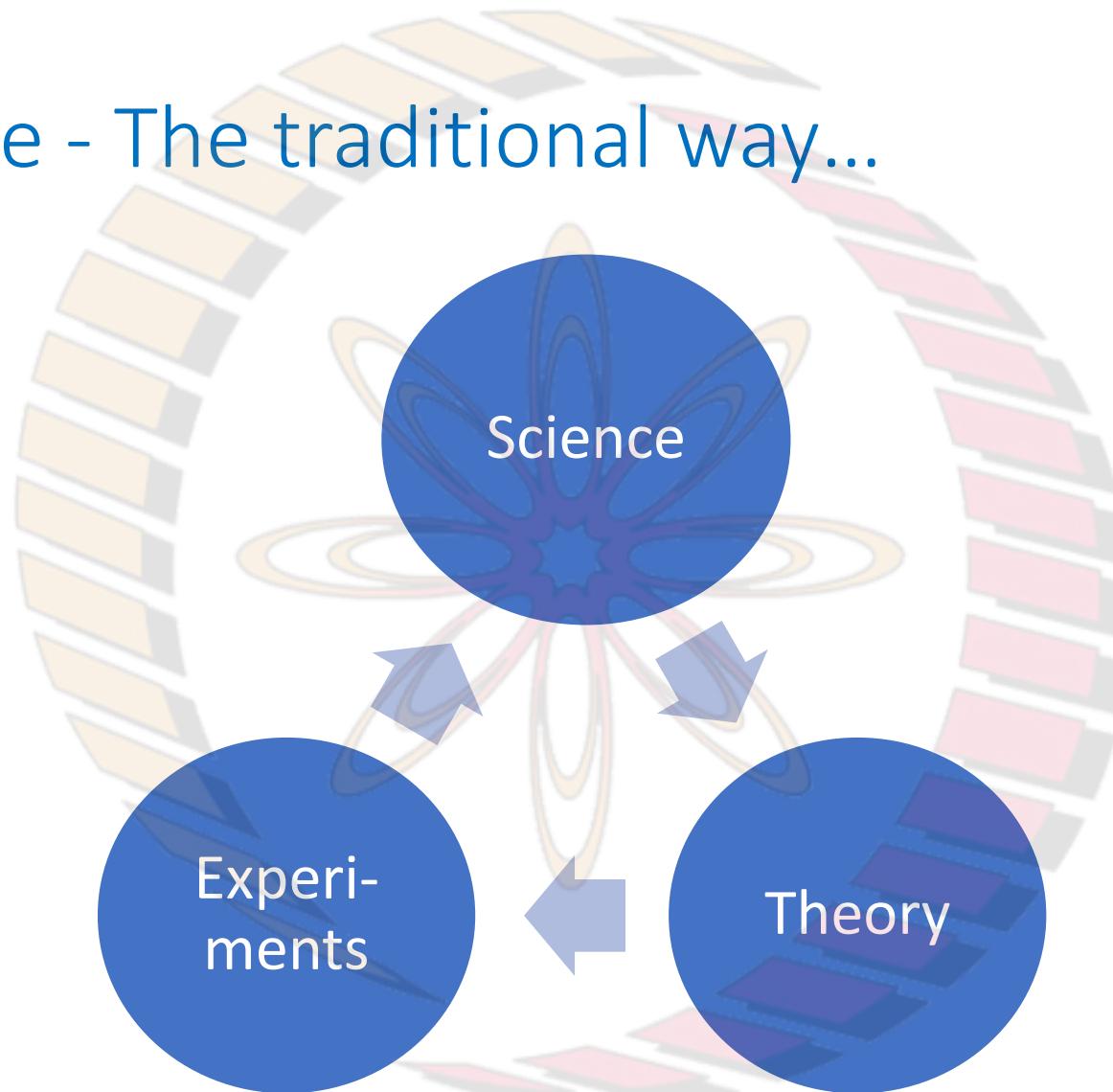
Performance Development over the years



- The Frontier system at Oak Ridge National Laboratory in Tennessee, USA is the most powerful system with an HPL score of 1.206 EFlop/s.
- It has a total of 8,699,904 combined CPU and GPU cores

Source: www.top500.org

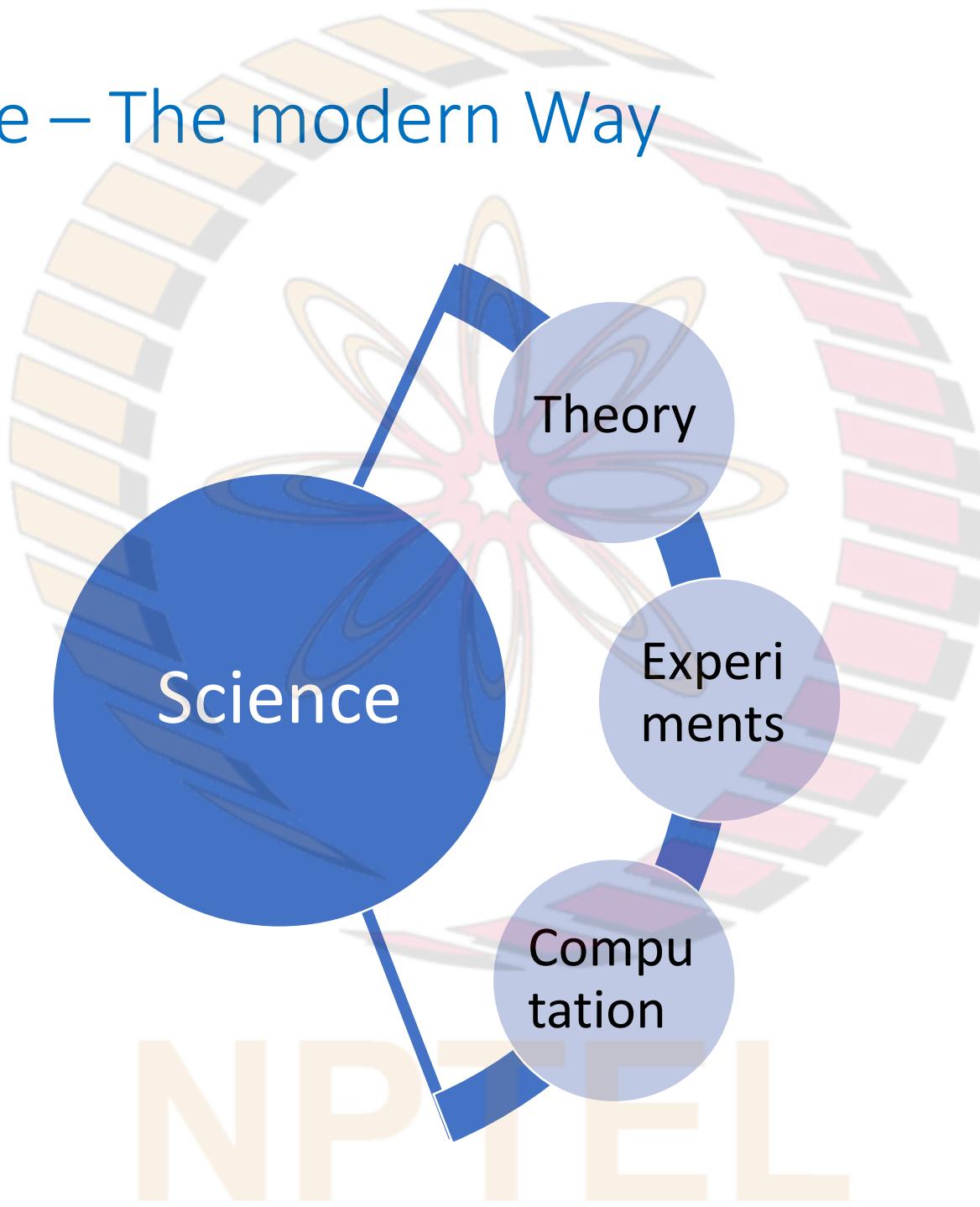
Doing science - The traditional way...



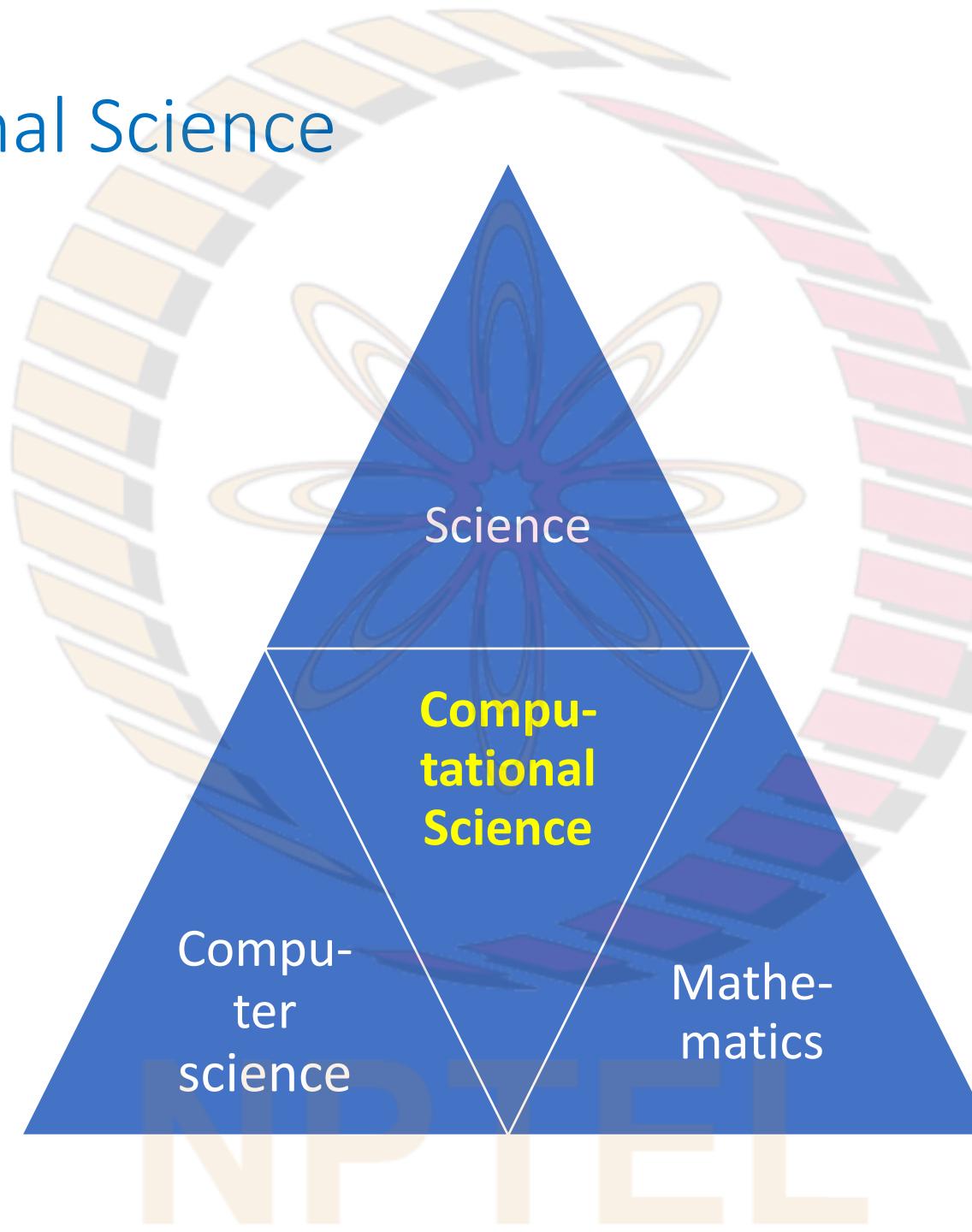
Mathematics is the alphabet with which God has written the universe.

- Galileo Galilei

Doing science – The modern Way



Computational Science



What is HPC

- High Performance Computing is a set of Computing technologies uses for
 - Very fast numeric simulation, modeling and data processing
- It makes use of parallel processing for running advanced application programs
- It is employed for specialised applications that require lot of mathematical calculations
- It uses the available computer power to execute a few applications extremely fast

A supercomputer is a system that performs at or near the currently highest operational rate for computers.

Parallel Computing Basics

- **Principle:** Large problems can often be divided into smaller ones, which are then solved concurrently
- **Parallel Processing:** Solving a task by making simultaneous use of multiple processing elements
- **Distributed Computing:** Solving a task by simultaneous use of multiple processing elements, typically isolated and heterogeneous in nature



Need for HPC

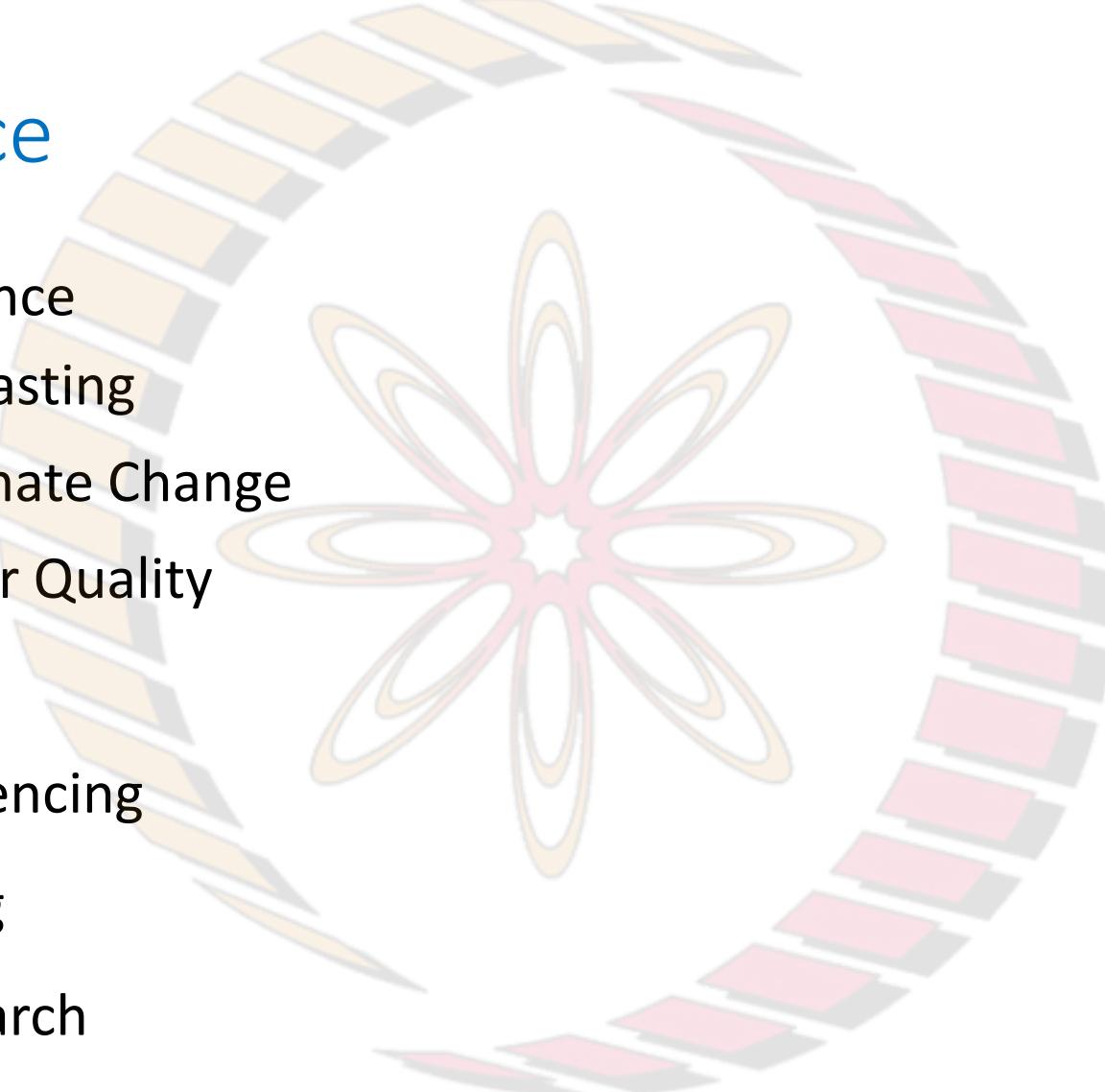
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Need for HPC

- Day to day life
 - Weather forecasting and early warnings
 - Improving healthcare
- Science
 - Investigating electronic structures
 - Exploring universe
- Engineering
 - Simulation before manufacturing
 - Designing safe structures – Analysis before construction

HPC in Science

- Atmospheric Science
 - Weather Forecasting
 - Combating Climate Change
 - Investigating Air Quality
- Life Science
 - Genome Sequencing
 - Drug Designing
 - Covid-19 Research



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HPC in Engineering

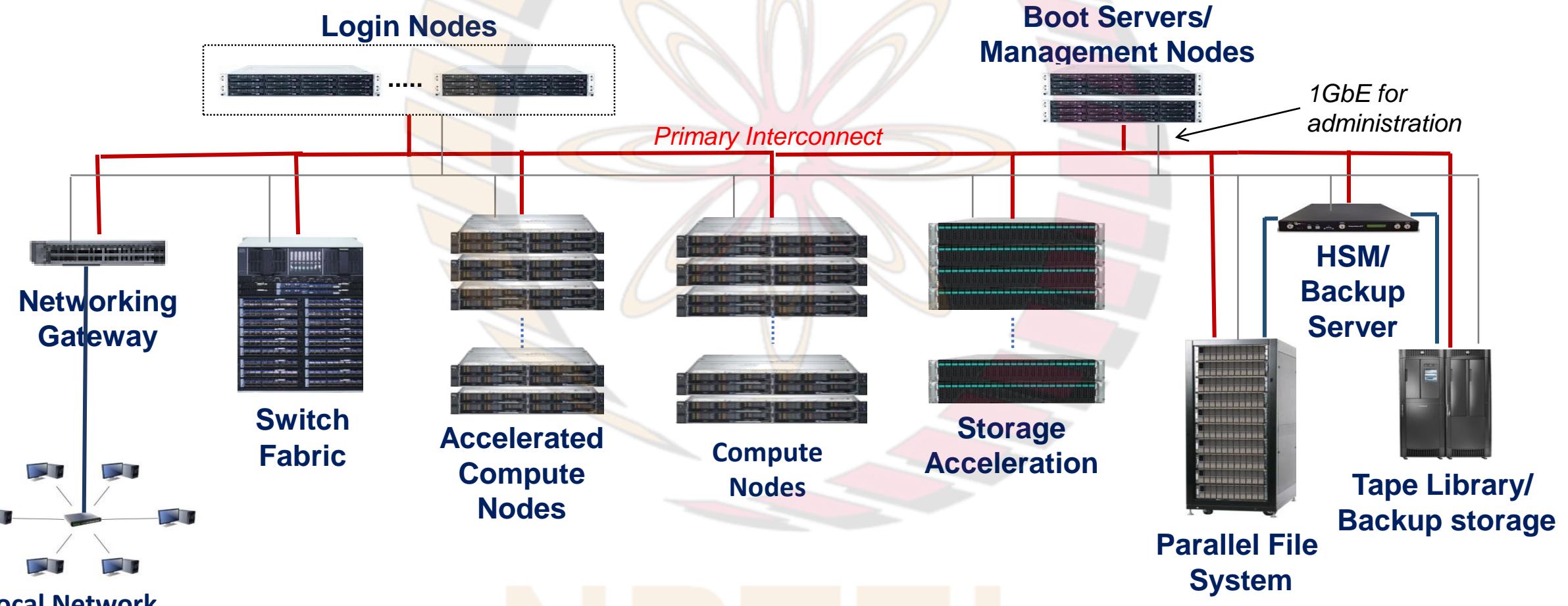
- Crash Simulation
 - Testing safety of automobile designs
- Aerodynamics Simulation
 - Design of aircrafts and missiles using Computational Fluid Dynamic techniques
- Structural Analysis
 - Design validation of civil structures' designs using Finite Element Analysis



Architecting a Supercomputing System

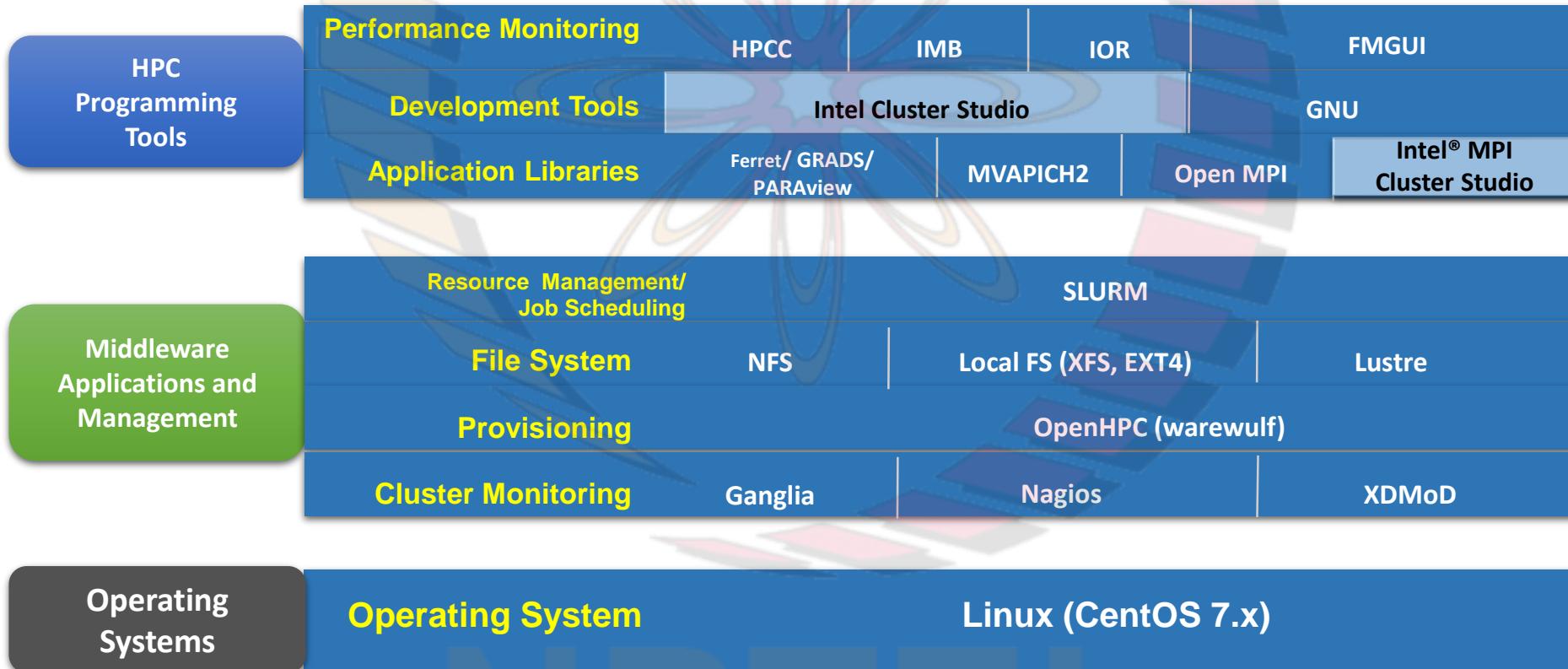
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Components of a Cluster



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HPC Software Stack



Components of Supercomputers

- Processors
- Memory
- Interconnects – Systems Area Networks
- Accelerators/Co-processors
- Storage subsystems – hardware, s/w - Parallel File Systems
- System Software
 - OS, Compiler
 - Parallel processing : MPI, Threads, Hybrid
 - Performance analysis and tuning, Debuggers
- Application software

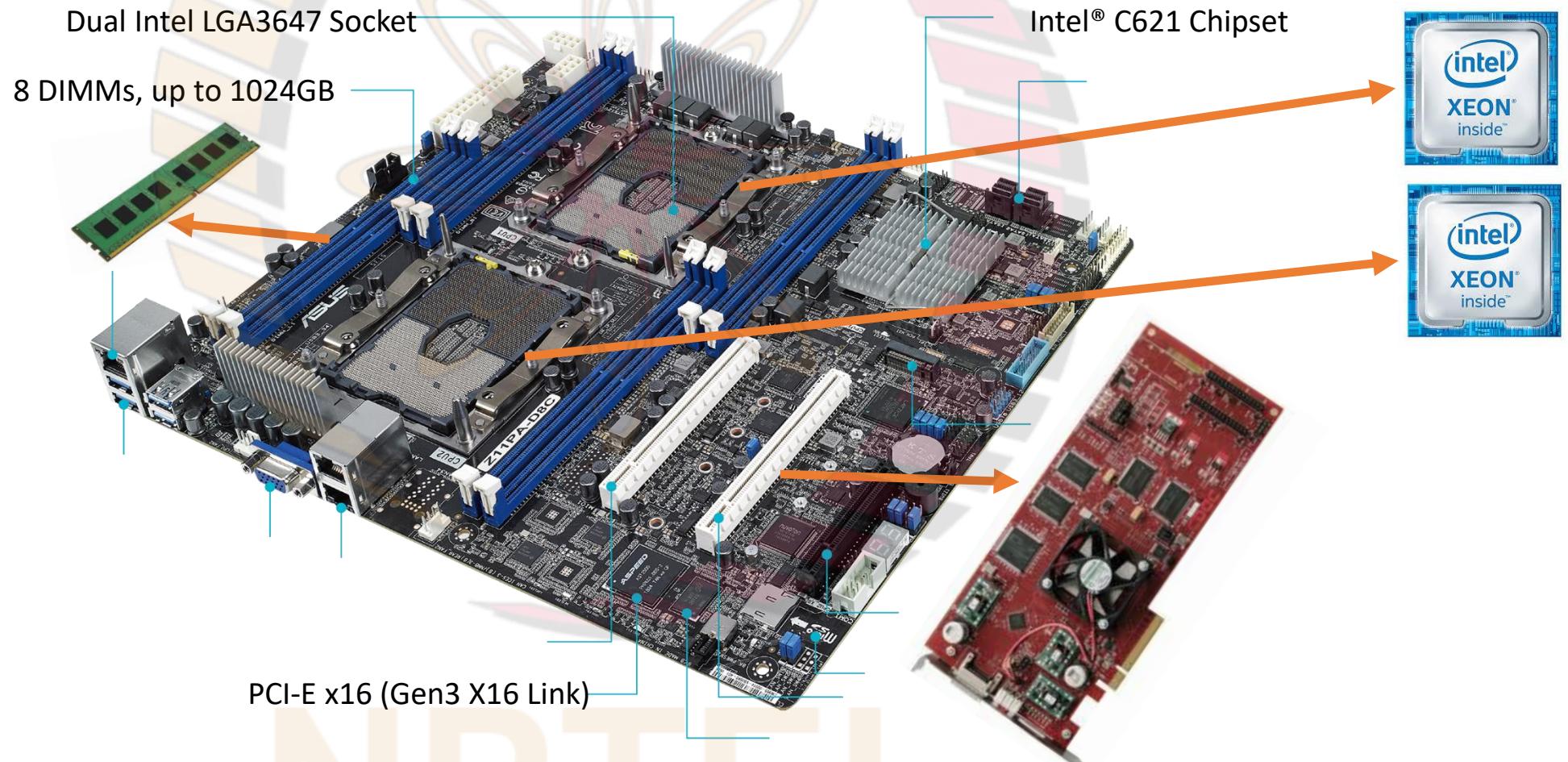
Rack mountable Server



Source: www.asus.com

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Dual socket Motherboard



Source: www.asus.com

Source: www.cdac.in

Source: www.intel.com

Advantages of Parallel Computing

- Overcome limitations of single CPU systems
 - Sequential systems are slow
 - Calculations may take days, weeks, years
 - More CPUs can get job done faster
 - Sequential systems are small
 - Data set may not fit in memory
 - More CPUs can give access to more memory
- The advantages thus, are
 - Save time
 - Solve bigger problems

Making use of HPC

- A team of domain experts and computational experts is needed to develop a HPC application
- Developing HPC aware software
 - Designing parallel algorithm
 - Writing parallel codes
 - Making use of parallel programming frameworks
- Making use of available applications and workflows
 - Open Source
 - Proprietary



Parallelization Methodology

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Desirable Attributes for Parallel Algorithms

- Concurrency
 - Ability to perform many actions simultaneously
- Scalability
 - Resilience to increasing processor counts
- Data Locality
 - High ratio of local memory accesses to remote memory accesses (through communication network)
- Modularity
 - Decomposition of complex entities into simpler components

Frameworks for Parallel Programming

- OpenMP
 - Works for shared memory computers
 - Compiler Directive based
- MPI
 - Suited for distributed memory computers
 - Makes use of MPI libraries
- OpenACC
 - Used for computers with accelerators
 - Compiler Directive based

Summary

- HPC is in use in our day to day life
 - Most of the times it is working silently
- HPC makes uses of parallel computing
- Clustering of nodes with appropriate communication network and software stack is the most common architecture in use today
- A Supercomputing cluster uses many other components other than the core compute nodes which has CPUs and GPUs
- Parallelization paradigm are the commonly used methods to achieve efficient parallelism
- Multiple frameworks are available for writing parallel programs



Thank You

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