Supercomputing: Why, What, and Where (are we) ?
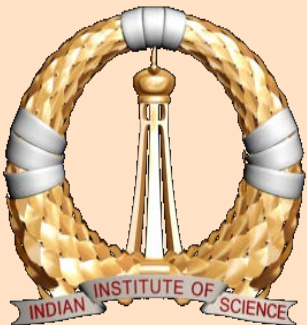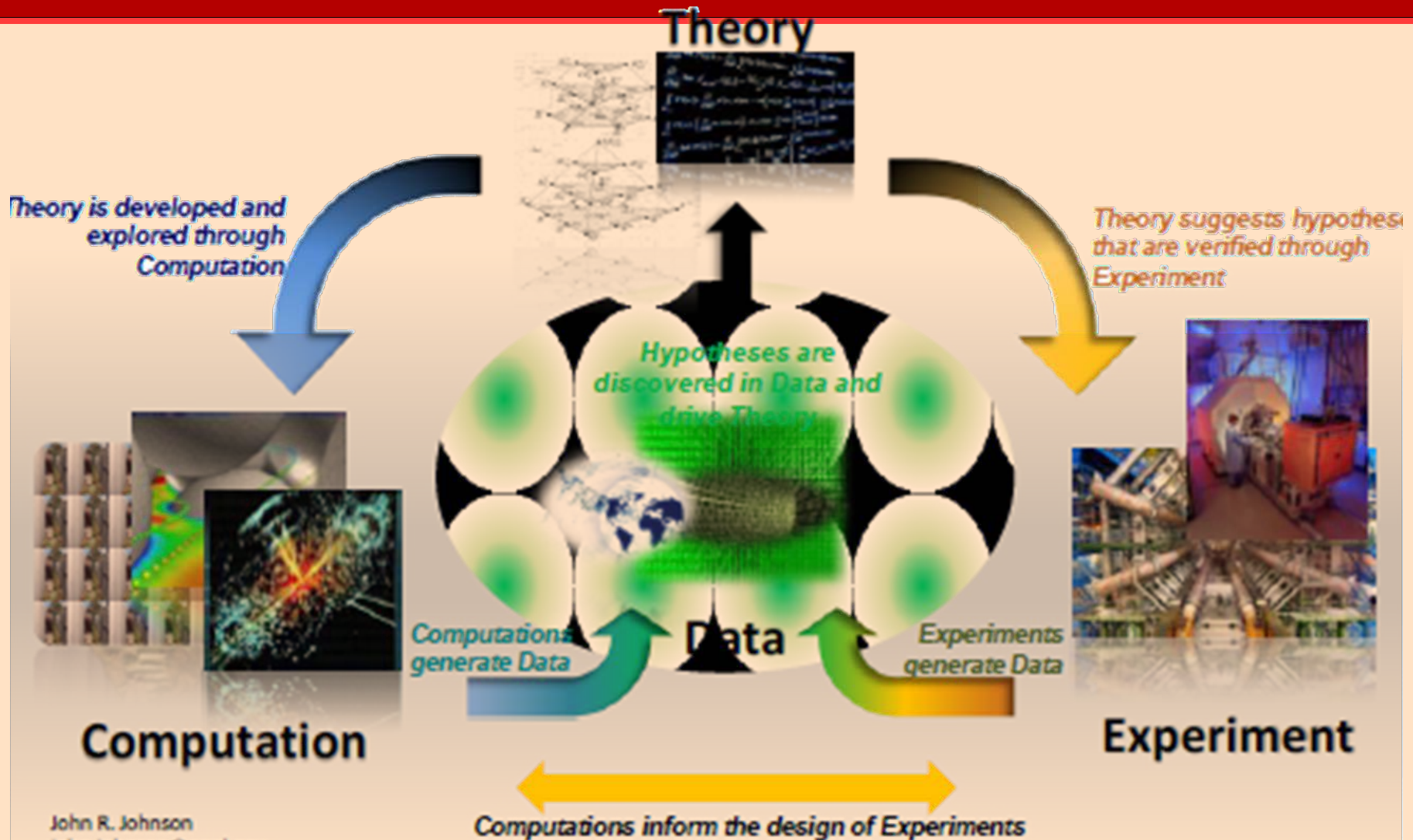
R. Govindarajan

Indian Institute of Science,
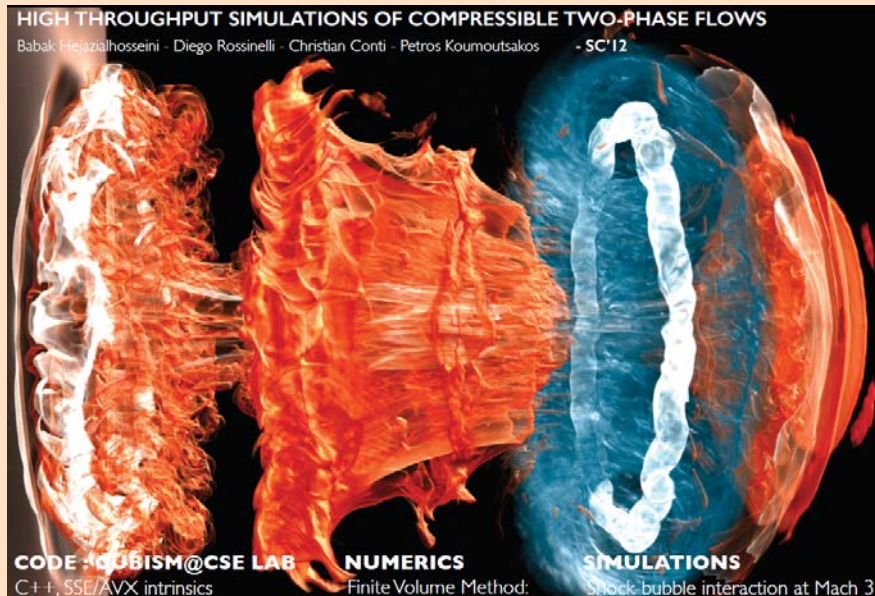Bangalore, INDIA
govind@serc.iisc.ernet.in

Third and Fourth Legs of Scientific Method
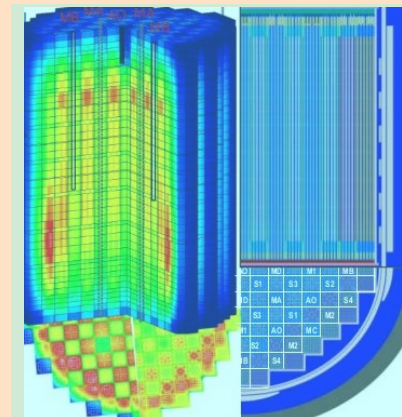
Supercomputing Applications

Computer Simulation
❑ **Abstract mathematical model mimicking dynamic behavior of components**
❑ **Conditions that cannot be easily or safely applied in real life**

HIGH THROUGHPUT SIMULATIONS OF COMPRESSIBLE TWO-PHASE FLOWS
Babak Hejazialhosseini · Diego Rossinelli · Christian Conti · Petros Koumoutsakos · SC'12

CODE : CUBISM@CSE LAB
C++, SSE/AVX intrinsics
NUMERICS
Finite Volume Method:
SIMULATIONS
Shock bubble interaction at Mach 3

Cosmic millennium -- Astrophysics
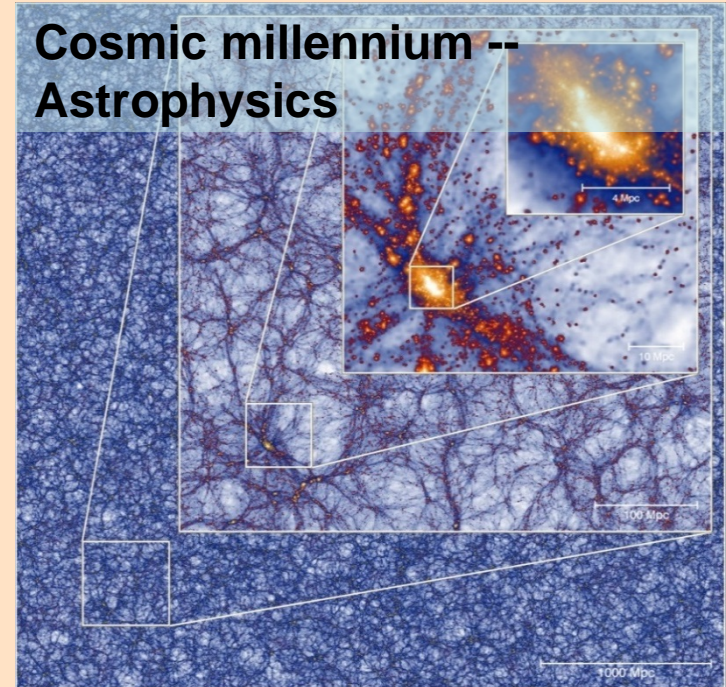
Nuclear Reactor Simulation
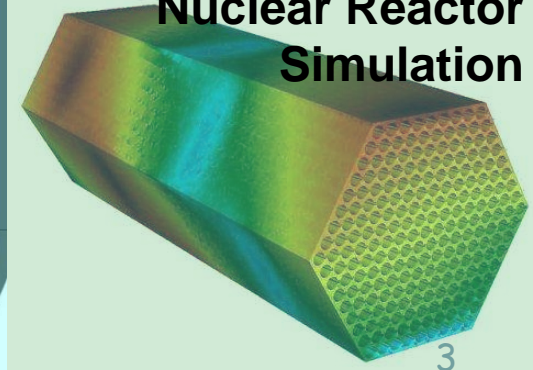
What is a Supercomputer?

- A hardware and software system that provides close to the maximum performance than can currently be achieved.

- What was a supercomputer a few (5) years ago, is probably an order of magnitude slower system compared to today's supercomputer system!

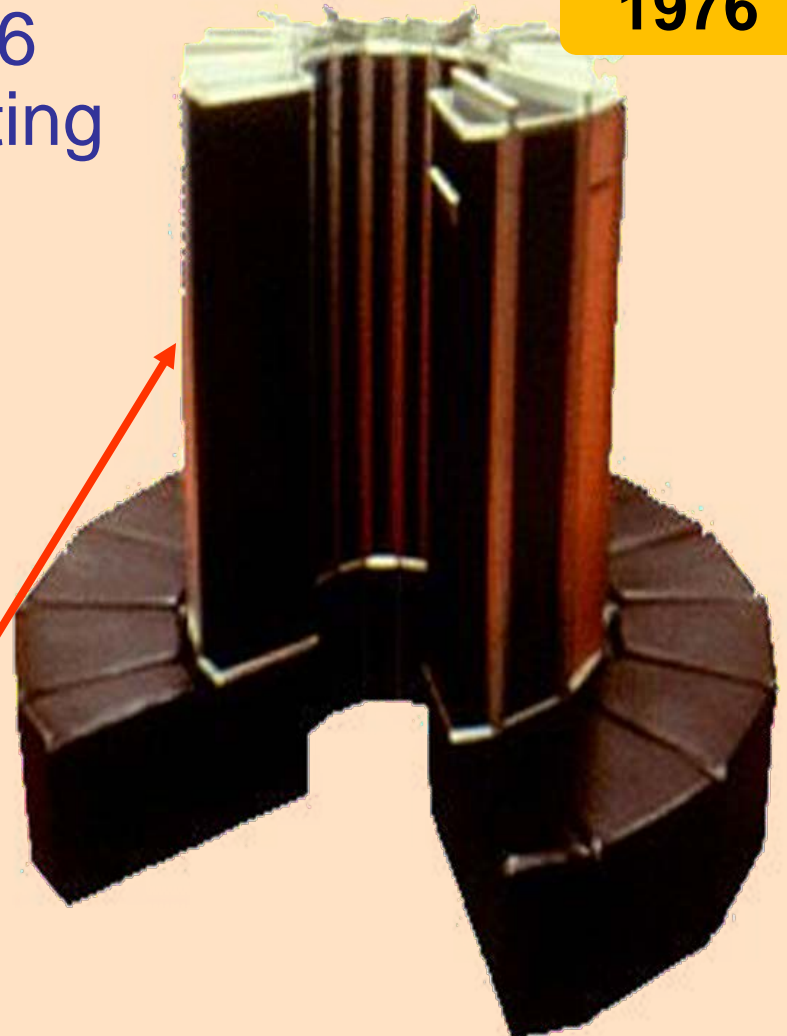Therefore, we use the term "high performance computing" also to refer to Supercomputing!

Era of Supercomputing

- Introduction of Cray 1 in 1976 ushered era of Supercomputing
  - Shared memory, vector processing
  - Good software environment
  - A few 100 MFLOPS peak
  - Cost about $5 million

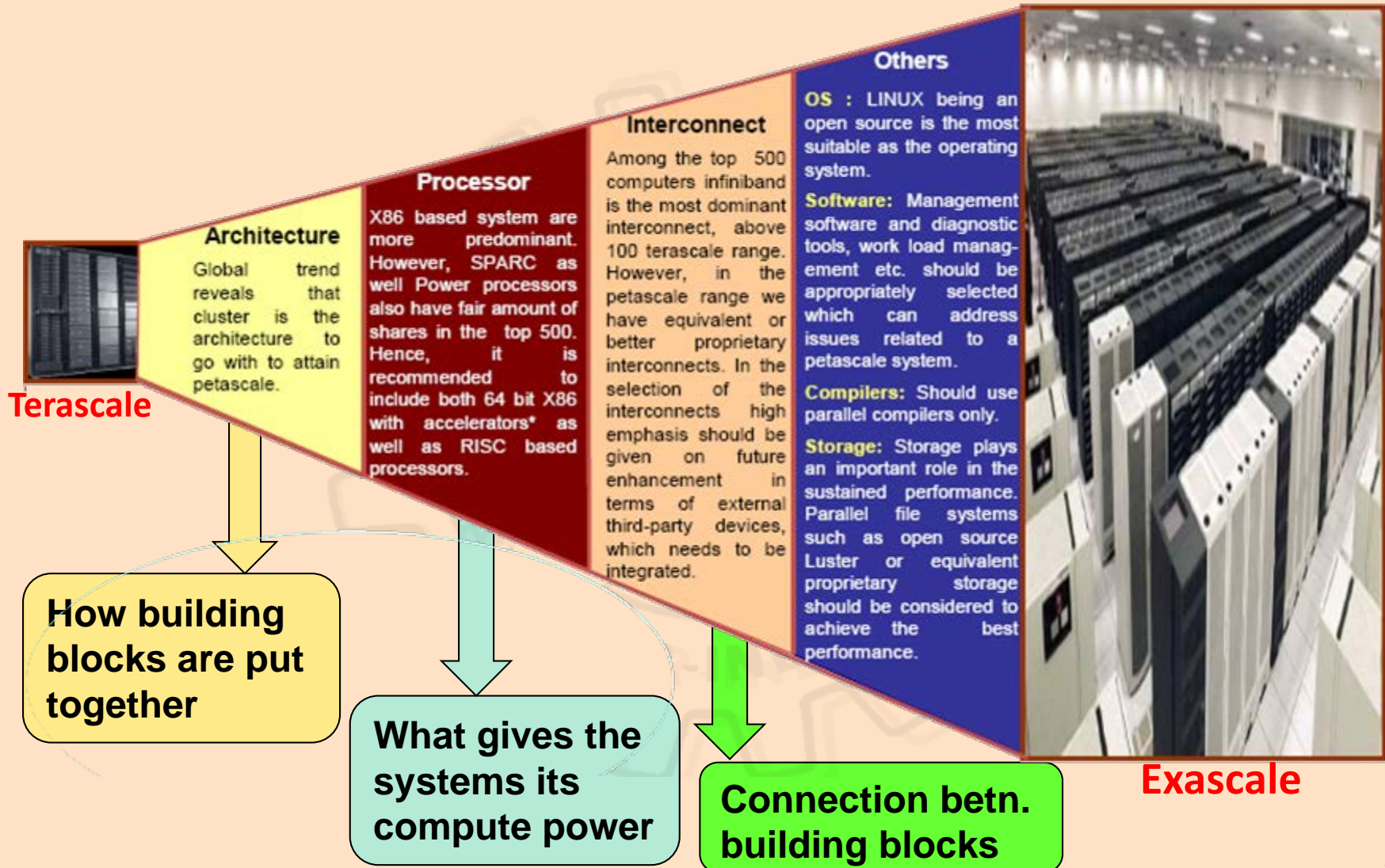**Apple1 iPhone 2007**

Performance of Supercomputer

- What are the top 10 or top 500 computers?
  - www.top500.org
  - Updated every 6 months
  - Measured using Rmax of Linpack   (solving $Ax = b$)
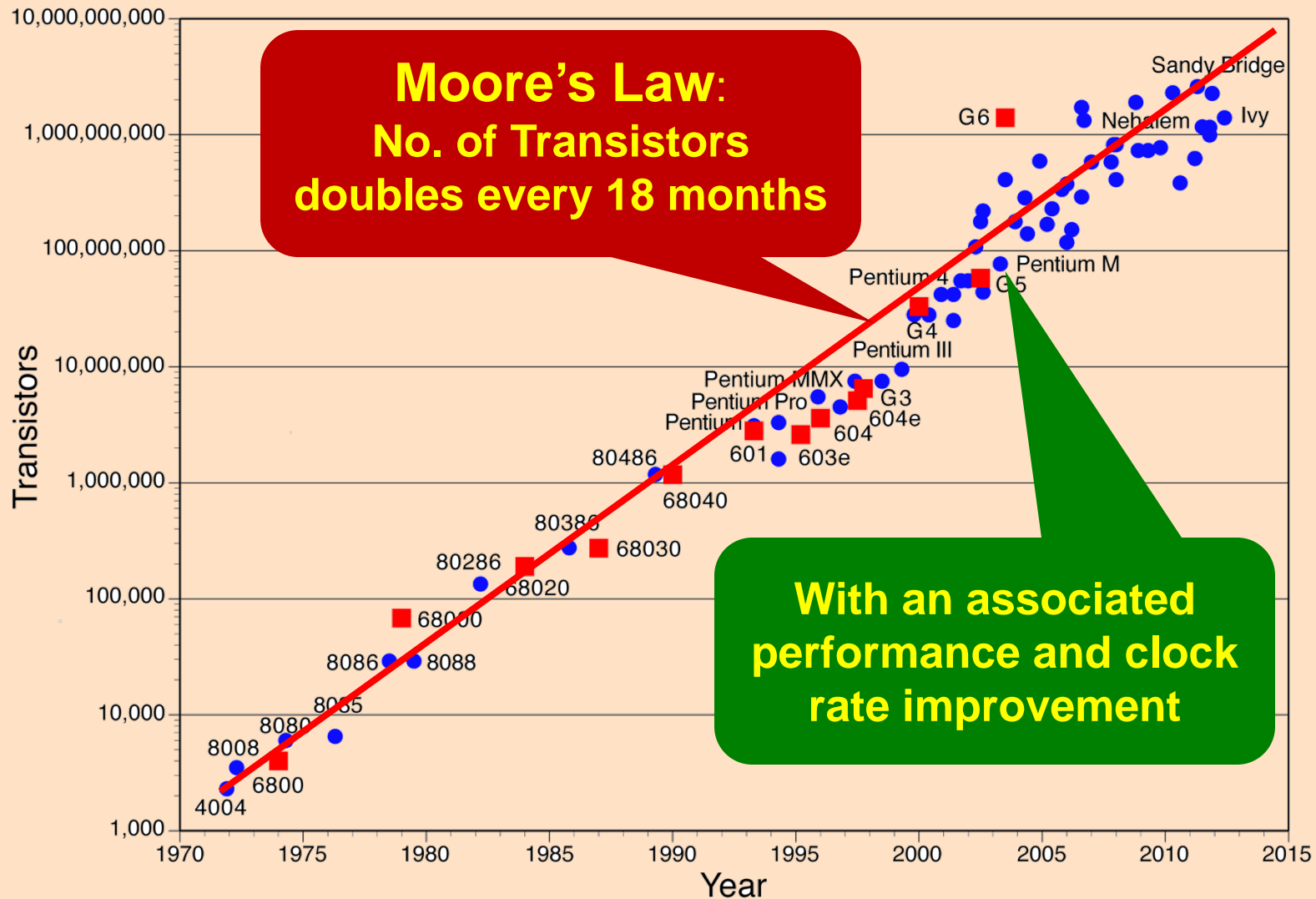- What is the trend?

Year	Performance (GFLOPS)	
	#1	
1993	59.7	0.422
2016	93,014,600	286,100

1,558,000 x Impr.!!

~10,649,600 processors!

Components of a Supercomputer

Terascale

Architecture

Global trend reveals that cluster is the architecture to go with to attain petascale.

Processor

X86 based system are more predominant. However, SPARC as well Power processors also have fair amount of shares in the top 500. Hence, it is recommended to include both 64 bit X86 with accelerators* as well as RISC based processors.

Interconnect

Among the top 500 computers infiniband is the most dominant interconnect, above 100 terascale range. However, in the petascale range we have equivalent or better proprietary interconnects. In the selection of the interconnects high emphasis should be given on future enhancement in terms of external third-party devices, which needs to be integrated.

Others

OS : LINUX being an open source is the most suitable as the operating system.

Software: Management software and diagnostic tools, work load management etc. should be appropriately selected which can address issues related to a petascale system.

Compilers: Should use parallel compilers only.

Storage: Storage plays an important role in the sustained performance. Parallel file systems such as open source Luster or equivalent proprietary storage should be considered to achieve the best performance.

Exascale

How building blocks are put together

What gives the systems its compute power

Connection betn. building blocks

What fuels this growth?

Moore's Law:
No. of Transistors
doubles every 18 months

With an associated performance and clock rate improvement

Source: Univ. of Wisconsin

The TOP 500 (June 2016)

Rank	Site	Manufacturer	Computer	Country	Cores	Rmax [Pflops]	Power [MW]
1	National SuperComputer Center in Wux	NRCPC	Sunway TaihuLight Sunway SW26010, 260C, 1.45 GHz	China	10,649,600	93.01	15.37
2	National SuperComputer Center in Tianjin	NUDT	Tianhe-2, NUDT TH MPP, Xeon E5 2691 and Xeon Phi 31S1	China	3,120,000	33.86	17.80
3	Oak Ridge National Labs	Cray	Titan Cray XK7, Opteron 6274 (2.2GHz) + NVIDIA Kepler K-20	USA	560,640	17.59	8.20
4	Lawrence Livermore Labs	IBM	Sequoia – BlueGene/Q	USA	1,572,864	17.17	7.89
5	RIKEN Advanced Institute for Computational Science	Fujitsu	K Computer SPARC64 VIIIfx 2.0GHz, Tofu Interconnect	Japan	705,024	10.51	12.66
6	DOE/SC/ANL	IBM	BlueGene/Q Power BQC 16C/1.6 GHz	USA	786,432	8.58	3.94
7	DOE/NNSA/ANL	Cray	Trinity Cray XC-40, Xeon E5-2698 16C (2.3GHz) Aries Interconnect	USA	301,056	8.10	
8	Swiss National Supercomputing	Cray	PizDaint Cray XC-30, Xeon E5-2670, 8C (2.6GHz) + NVIDIA K20x	USA	115,984	6.27	2.32

Top 500 June 2016 List : www.top500.org

TOP500 Supercomputers by Country

India
5 – 10 systems

Legend:
United States, Japan, Germany, United Kingdom, France, China, Italy, Canada, Korea, South, Sweden, Switzerland, Netherlands, Australia, India, Russia, Spain, Saudi Arabia, Norway, Brazil, Taiwan, Finland, Poland, Denmark, Mexico, Belgium, Austria, Israel, New Zealand, Hong Kong, Singapore, Malaysia, South Africa, Egypt, Portugal, Luxembourg, Slovenia, Ireland, Greece, Thailand, Turkey, Hungary, Bulgaria, Venezuela, United Arab Emirates, Indonesia, Belarus, Vietnam, Slovak Republic, Philippines, Oman, Liechtenstein, Czech Republic

TOP500 Date

10

TOP SUPERCOMPUTERS INDIA

Rank	Site	System	Cores/Processor Sockets/Nodes	Rmax (TFlops)	Rpeak (TFlops)
1	Supercomputer Education and Research Centre (SERC), Indian Institute of Science (IISc), Bangalore	Cray XC-40 Cluster (1468 Intel Xeon E5-2680 v3 @ 2.5 GHz dual twelve-core processor CPU-only nodes, 48 [Intel Xeon E5-2695v2 @ 2.4 Ghz single twelve-core processor+Intel Xeon Phi 5120D] Xeon-phi nodes, 44 [Intel Xeon E5-2695v2 @ 2.4 Ghz single twelve-core processor+NVIDIA K40 GPUs] GPU nodes) w/ Cray Aries Interconnect. HPL run on only 1296 CPU-only nodes. OEM: Cray Inc., Bidder: Cray Supercomputers India Pvt. Ltd.	36336C + 2880ICO + 126720G/ 3028C + 48ICO + 44G/ 1560C + 48ICO + 44G	901.51 (CPU-only)	1244.00 (CPU-only)
2	Indian Institute of Tropical Meteorology, Pune	IBM/Lenovo System X iDataPle DX360M4, Xeon E5-2670 8C 2.6 GHz, Infiniband FDR OEM: IBM/Lenovo, Bidder: IBM India Pvt. Ltd.	38016/ /	719.2	790.7
3	Indian Lattice Gauge Theory Initiative, Tata Institute of Fundamental Research (TIFR), Hyderabad	Cray XC-30 cluster (Intel Xeon E5-2680 v2 @ 2.8 GHz ten-core CPU and 2688-core NVIDIA Kepler K20x GPU nodes) w/Aries Interconnect OEM: Cray Inc., Bidder: Cray Supercomputers India Pvt. Ltd.	4760C + 1279488G/ 476C + 476G/ 476C + 476G	558.7	730.00
4	Indian Institute of Technology, Delhi	HP Proliant XL230a Gen9 and XL250a Gen9 based cluster (Intel Xeon E5-2680v3 @ 2.5 GHz dual twelve-core CPU and dual 2880-core NVIDIA Kepler K40 GPU nodes) w/Infiniband OEM: HP, Bidder: HP	10032C + 927360G/ 836C + 322G/ 418C + 161G	524.40	861.74
5	Center for Development of Advanced Computing (C-DAC), Pune	Param Yuva2 System (Intel Xeon E5-2670 (Sandy Bridge) @ 2.6 GHz dual octo-core CPU and Intel Xeon Phi 5110P dual 60-core co-processor nodes) w/Infiniband FDR OEM: Intel, Bidder: Netweb Technologies	3536C + 26520 ICO/ 442C + 442 ICO/ 221C + 221 ICO	388.44	520.40
6	CSIR Fourth Paradigm Institute (CSIR-4PI), Bangalore	HP Cluster Platform 3000 BL460c (Dual Intel Xeon 2.6 GHz eight core E5-2670 w/Infiniband FDR) OEM: HP, Bidder: HCL Infosystems Ltd.	17408/2176/1088	334.38	362.09
7	National Centre For Medium Range Weather Forecasting, Noida	IBM/Lenovo System X iDataPlex DX360M4, Xeon E5-2670 8C 2.6 GHz, Infiniband FDR OEM: IBM/Lenovo, Bidder: IBM India Pvt. Ltd.	16832/ /	318.4	350.1
8	Indian Institute of Technology, Kanpur	Cluster Platform SL230s Gen8, Intel Xeon E5-2670v2 10C 2.5 GHz, Infiniband FDR. OEM: HP, Bidder: HP	15360/1536/768	295.25	307.2

Supercomputers: Are they White Elephants ?

33.8   PFLOPS
3.12 M Cores
17.8 MW of power

THE FUTURE
>180 PFLOPS
(option to increase up to 450 PF)
>50,000 nodes
13MW
2018 delivery

93.0   PFLOPS
10.6   M Cores
15.3   MW of power

THE FUTURE

>180 PFLOPS
(option to increase up to 450 PF)

33.
3.
17

- ➢ Huge Investments
- ➢ Large maintenance & operational expenditure
- ➢ What can we do with them?
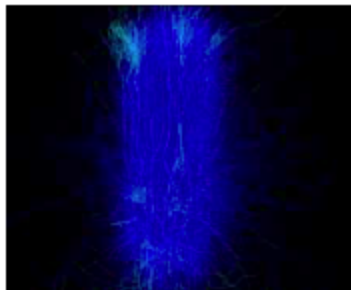- ➢ Are they the worth the investment/ cost?

93.0   PFLOPS
10.6   M Cores
15.3   MW of power

Blue Brain Project

BBP Phase I: Neocortical Column

Create a faithful "in silico" replica at cellular level of a neocortical column of a young rat by the means of:

- reverse engineering the biology components
- forward constructing functional mathematical models

- **Building**
  10,000 morphologically complex neurons
- **Constructing**
  a circuit with 30,000,000 dynamic synapses
- **Simulating**
  the column close to real-time
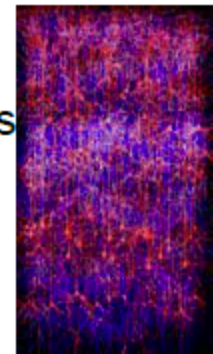
© Blue Brain Project

ÉCOLE POLYTECHNIQUE
FÉDÉRALE DE LAUSANNE

Blue Brain Project

BBP Phase I: Neocortical Column

Create a faithful "in silico" replica at cellular level of a neocortical

- **Modeling & understanding the brain (biological, physiological, neurological functioning)**

- **Comprehensive digital reconstruction to further refine, expand and validate newer models**

- **Diagnosing and treating brain diseases**

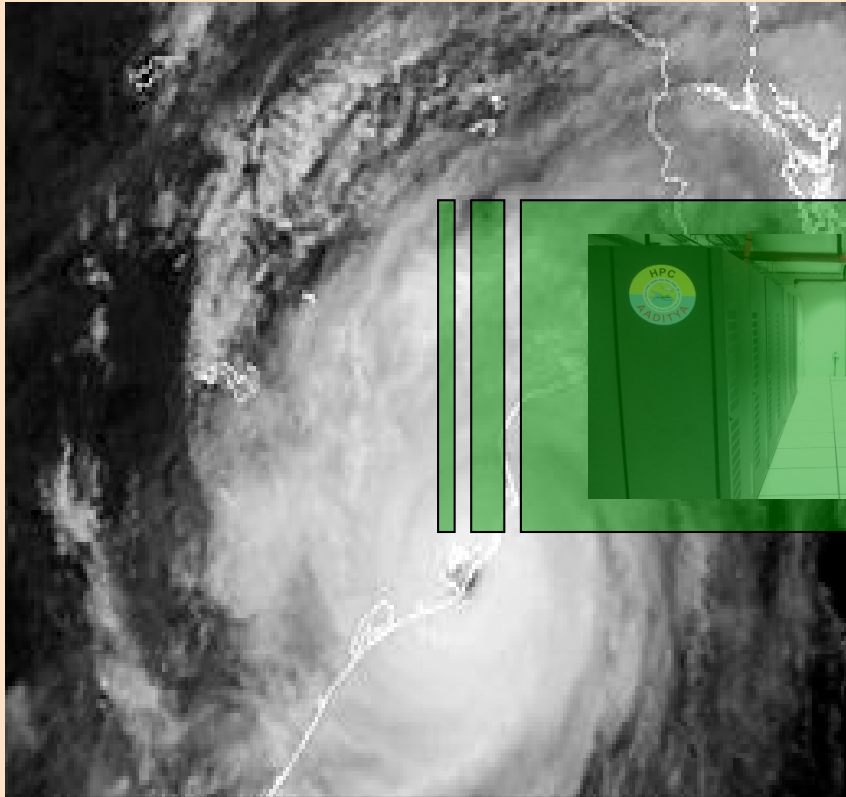- **Leading to new computing technology, neurobotic and neuromorphic computing**

ÉCOLE POLYTECHNIQUE
FÉDÉRALE DE LAUSANNE

Large Hadron Collider – Higgs Boson
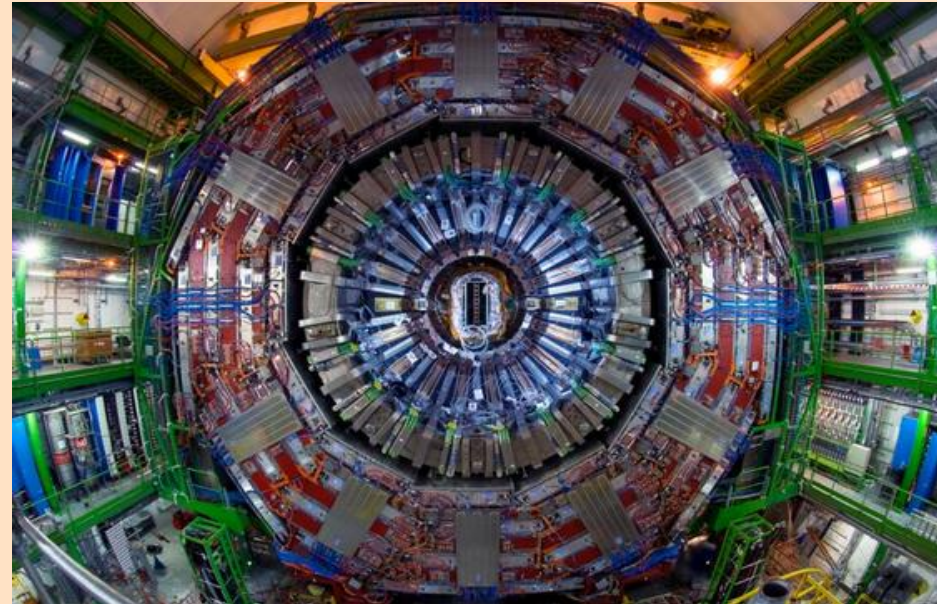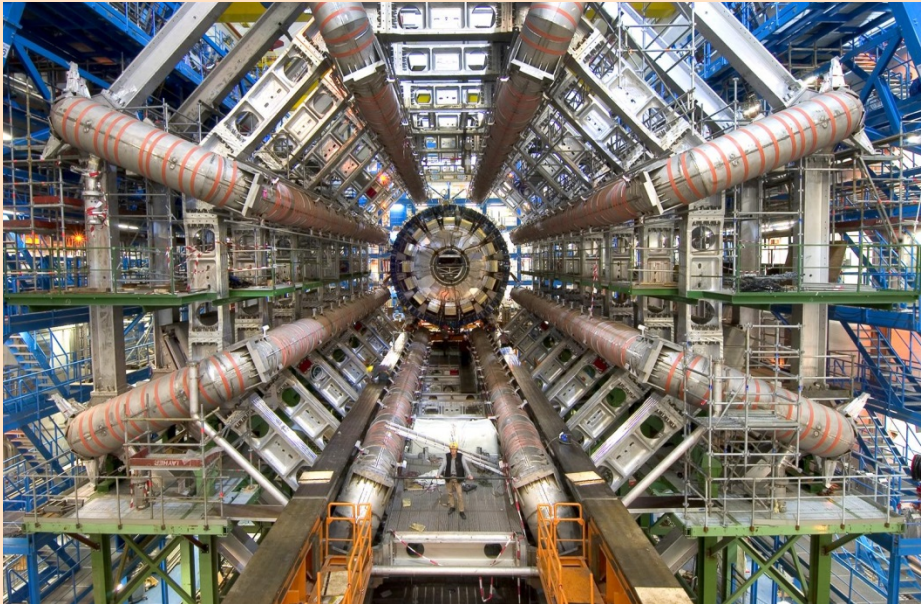
World LHC Compute Grid
Several 100,000 Cores, distributed across the world
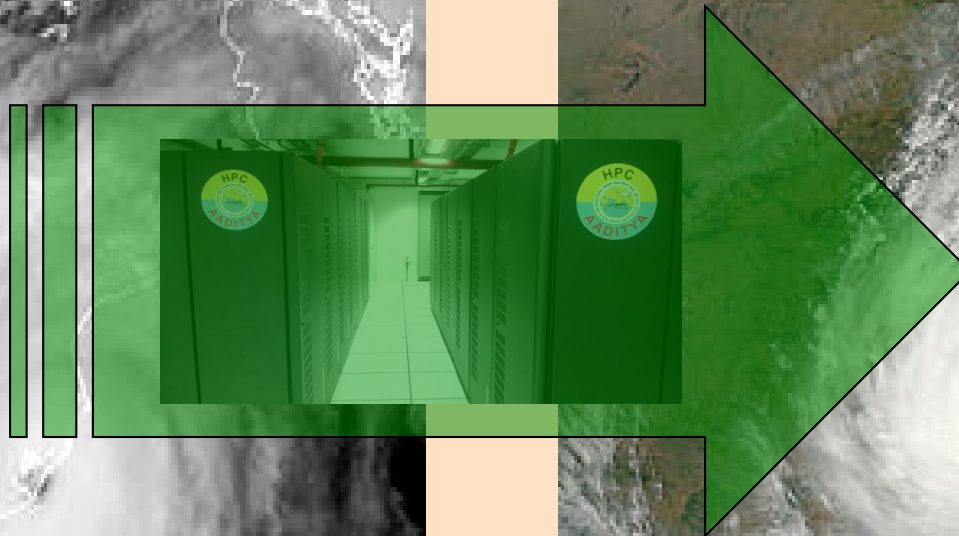Petabytes to exabytes of Data to be analysed and stored

Large Hadron Collider – Higgs Boson

Simulated Large Hadron Collider CMS particle detector data depicting a **Higgs boson** produced by colliding protons decaying into hadron jets and electrons
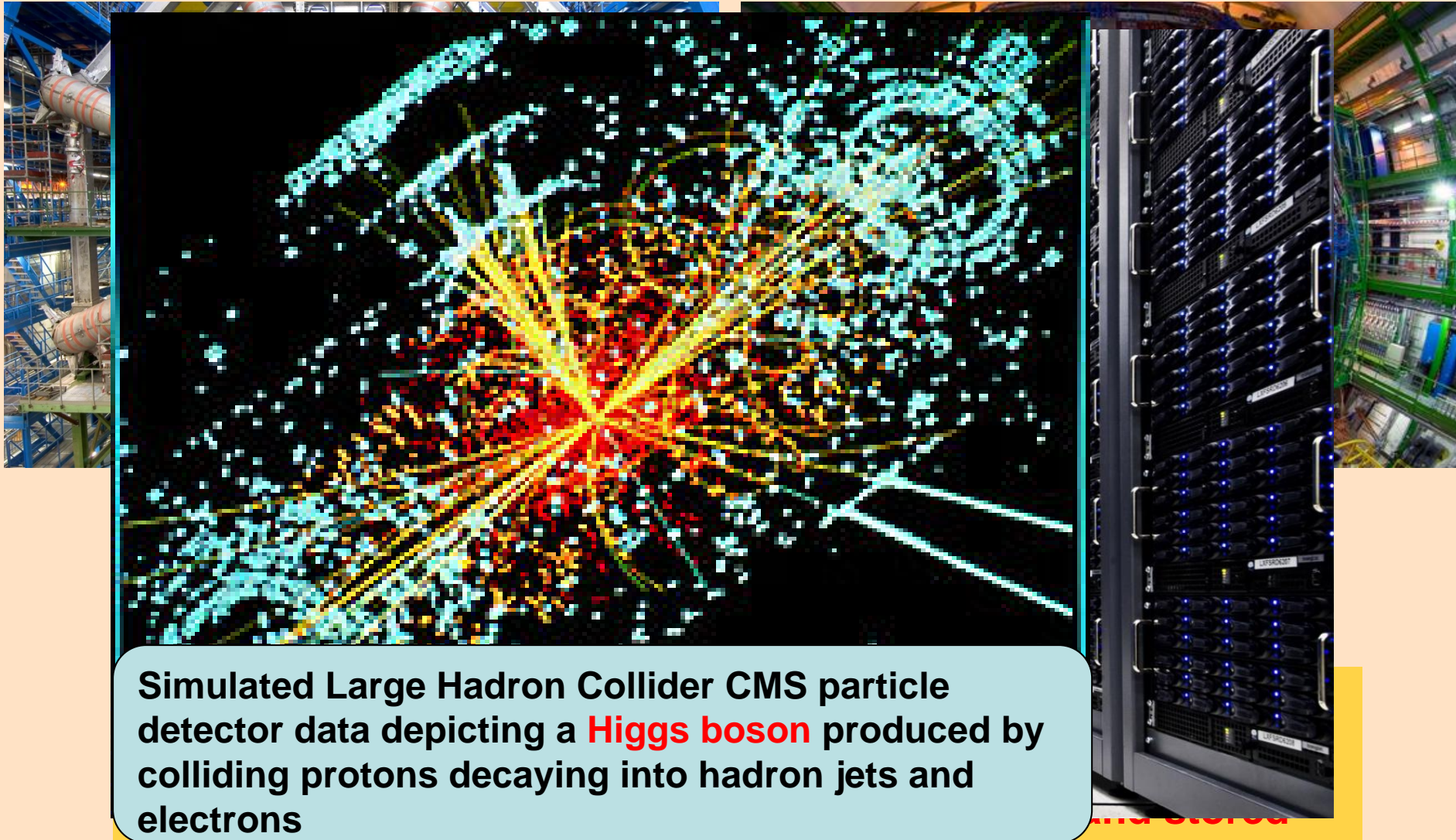
Societal Impact of Supercomputing

Cyclone 05B : Oct. 25, 1999
Category 5 (Extremely Severe)
10,000+ deaths
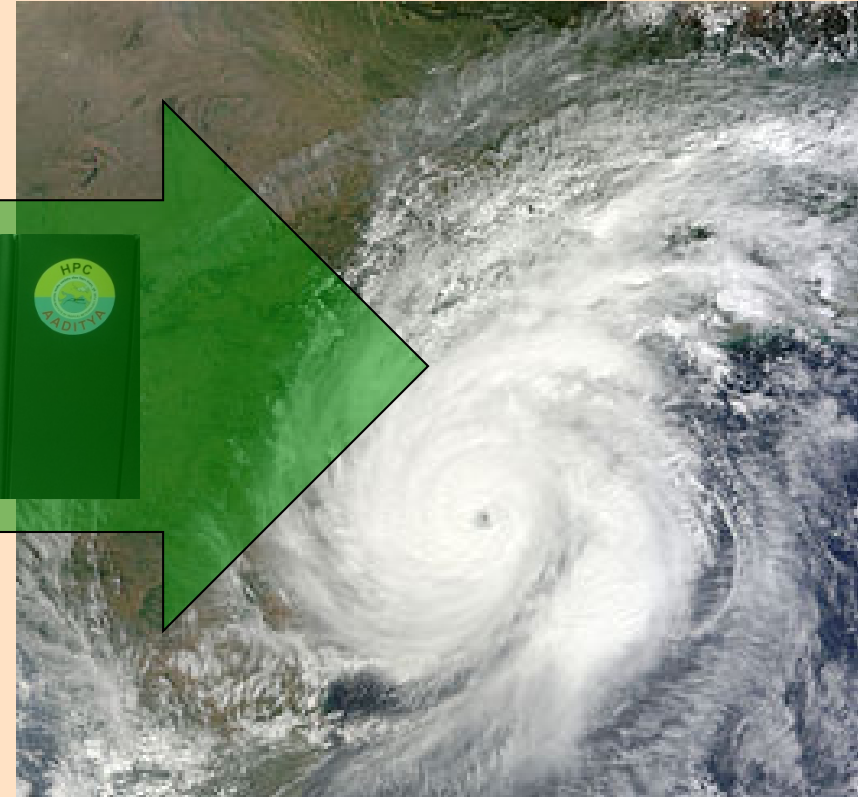
Cyclone Hudhud: Oct.12, 2014
Category 4 (Extremely Severe)
124 deaths

Hudhud: Spot on twice, India's Met Dept beats global weathermen hollow

Bhubaneswar: Others may have a more enviable international profile, but for the second time in the last one year, India Meteorological Centre (IMD) has proved that it has no peer when it comes to forecasting cyclonic storms in the Indian seas.

As it had done in the case of Cyclone Phailin exactly a year ago, IMD hit the bull's eye when it came to tracking the course of Cyclone Hudhud, assessing its intensity and predicting the place and timing of its landfall.

While even the US-based Joint Typhoon Warning Centre (JTWC), which is among the most trusted weather forecast stations in the world, got it all wrong, IMD was spot on with its prediction on Hudhud - not just about the place of the landfall (Vishakhapatnam), but also the timing (shortly before noon) and the velocity of wind accompanying it (170-180 km/hr, gusting up to 195 km/hr).
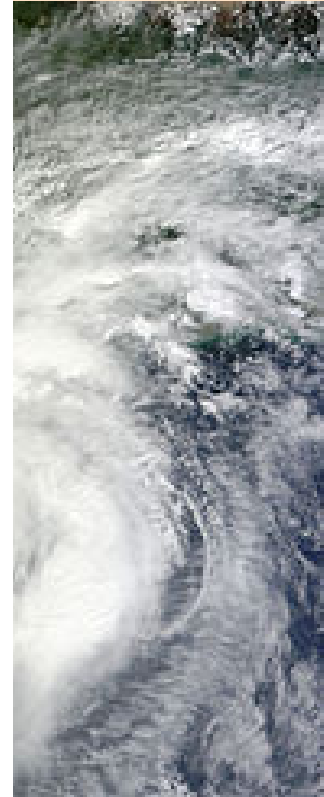
The importance of the accuracy of forecast of cyclonic storms — or any natural disaster for that matter — goes much beyond scoring brownie points or nationalistic breast-beating. It is the key to saving precious lives and preventing damage to property and public assets.

A comparison with the Super Cyclone that devastated the state in 1999 would put things in perspective.

Even after accounting for the fact that it was a storm of much greater intensity, it is hard to explain away the loss of close to 10, 000 human lives, over five lakh cattle and lasting damage to public infrastructure in the affected areas that is said to have pushed the back by a decade.
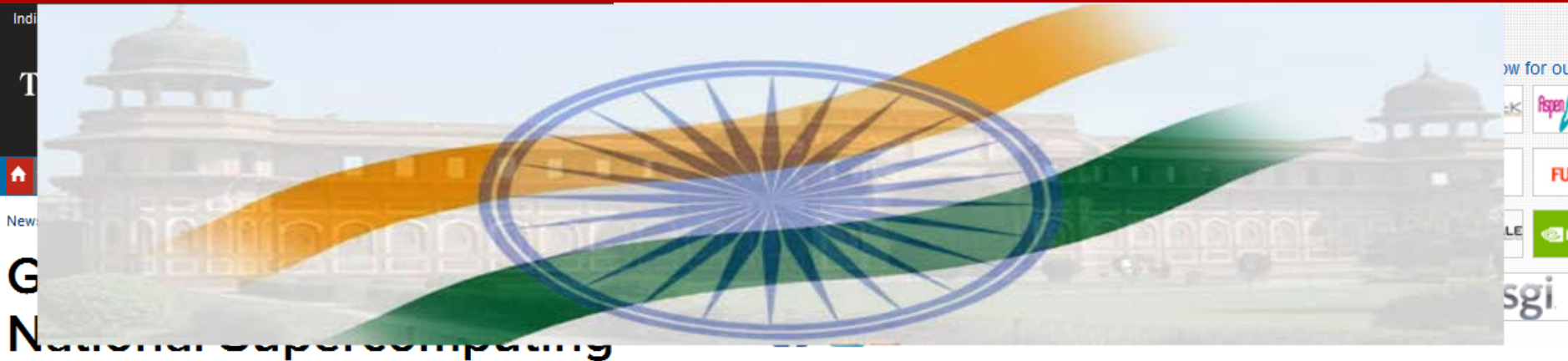
IMD's forecast on Cyclone Hudhud having proved remarkably accurate. AFP

Cyclone 05B
Category 5 (
10,000+ deat

.12, 2014
Severe)

19

Open Source Drug Discovery

OSDD is open innovation translational research platform for both computational and experimental technologies

Targets drugs for diseases like Tuberculosis, Malaria, etc.
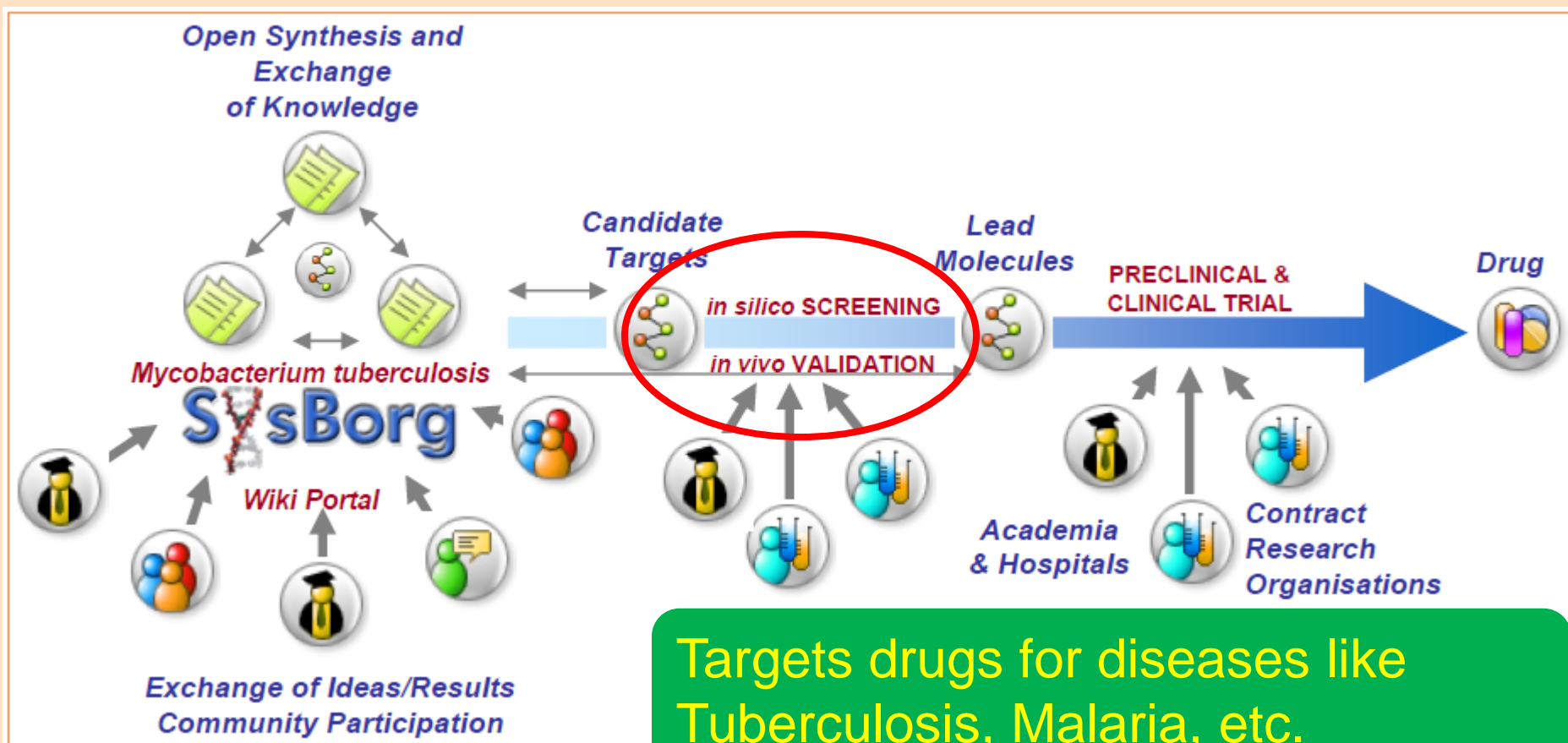
National Supercomputing Mission

PTI | Mar 27, 2015, 10.49 AM IST

October 6, 2014

India to Launch $730M National Supercomputing Mission

Tiffany Trader

India plans to become a world-class computer engine in the next... the national government launched a strategy to build a supercomputing grid, comprised of more than 70 high-performance computing fa... The project is expected to take seven years and comes with a price tag of $730 million (Rs. 4,500-crore). It calls for at least three petascale machines a... ut times r r th country's current record-holder, which puts ... est on of ... 2.5 0 petaflops range.

As reported by *HindustanTimes*, India's finance ministry panel authorized the National Supercomputing Mission, which is being jointly managed by the department of science and technology and the department of electronics and information technology. However, the project still has to clear the Indian cabinet before becoming official policy.

The Cabinet Committee on Economic Affairs has a... mo... of the mission that will enable India to lea... Read

Prime Minister Narendra Modi, has approved the launch of ... enable India to leapfrog to the league of world-class compu... official release said.
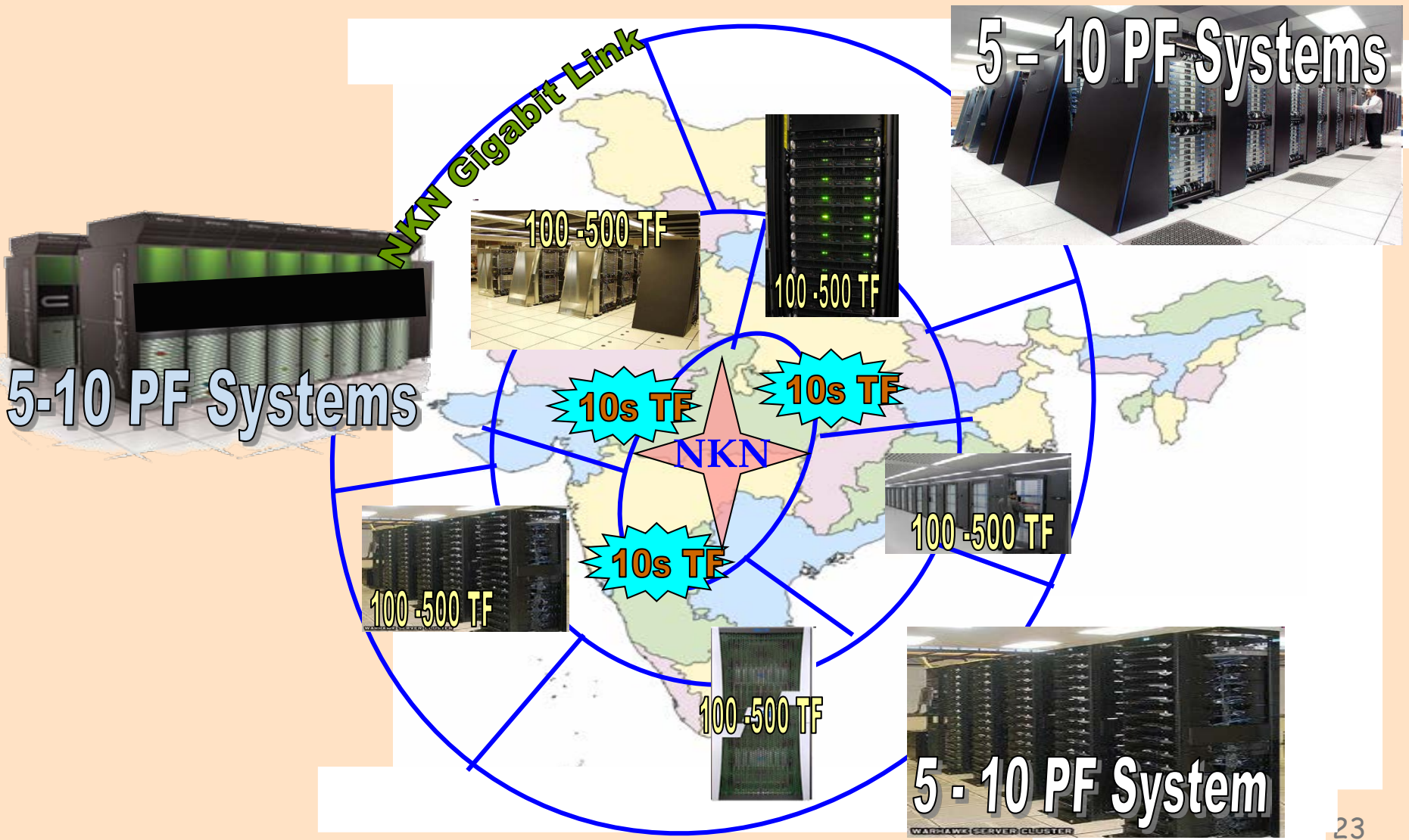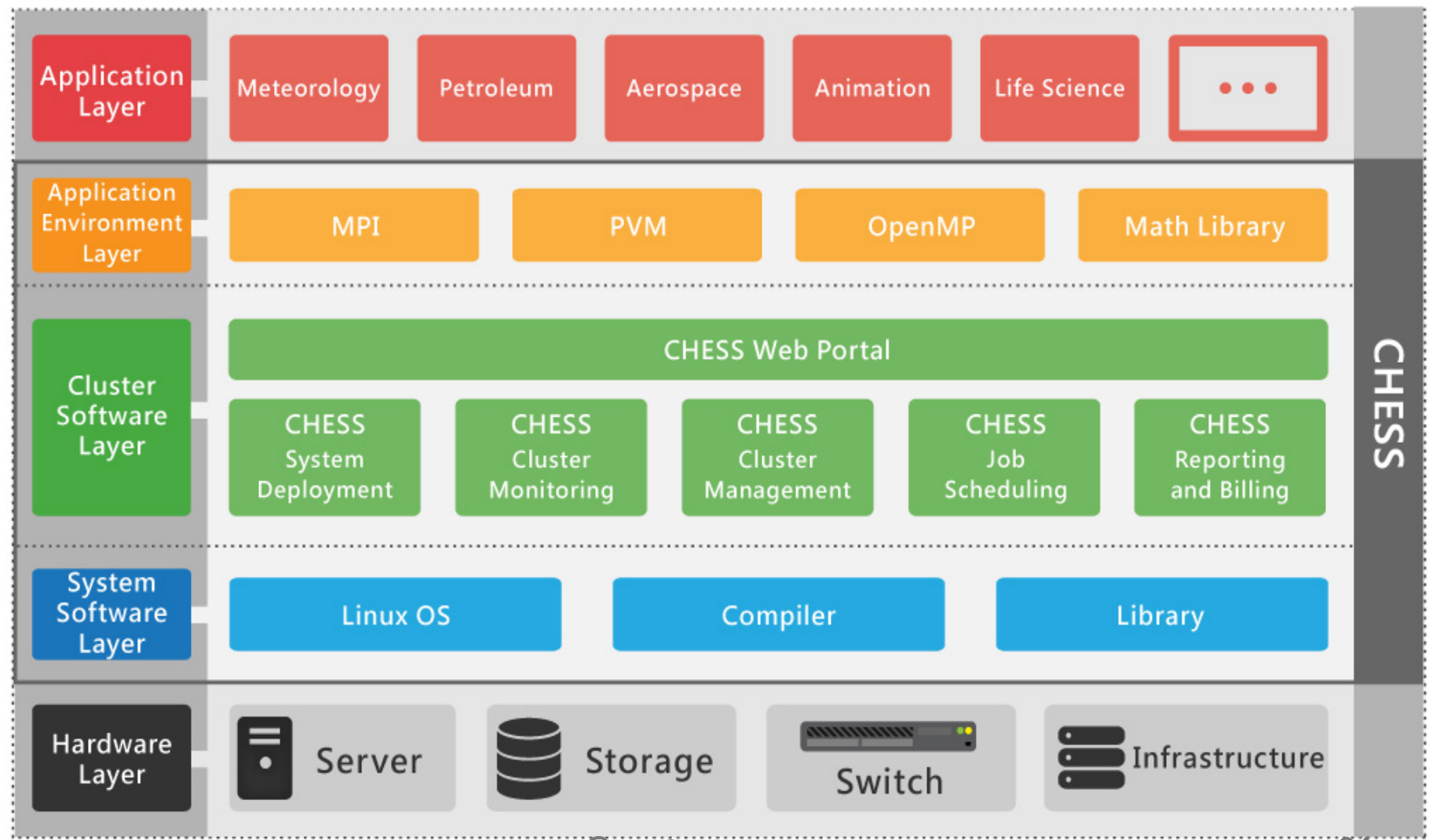
NSM Objectives

- Multi-tiered HPC Infrastructure
- Development of HPC applications
- HPC-aware Manpower Development
- Next generation R & D on HPC Systems

- **Implementing agencies : IISc and C-DAC**
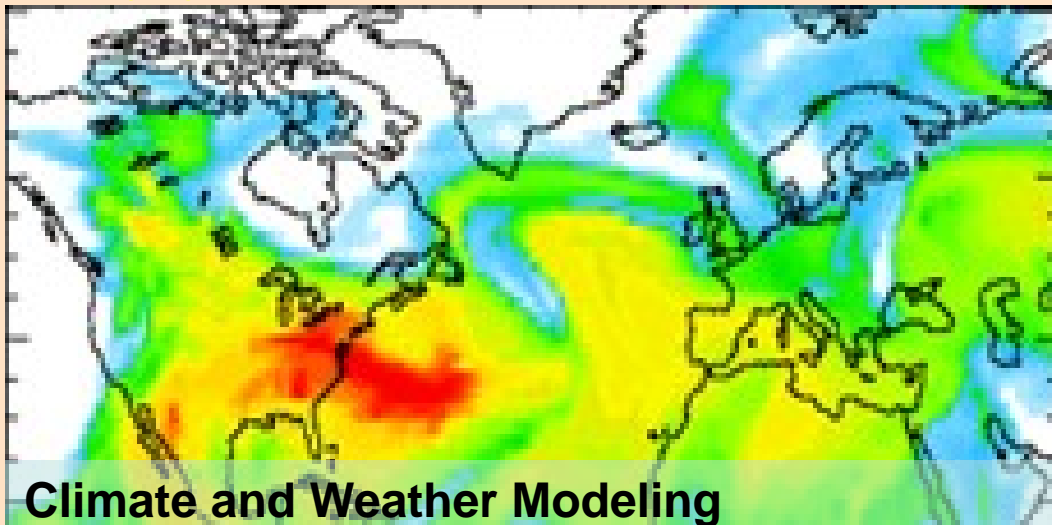
- **SERC will play a major role in NSM**
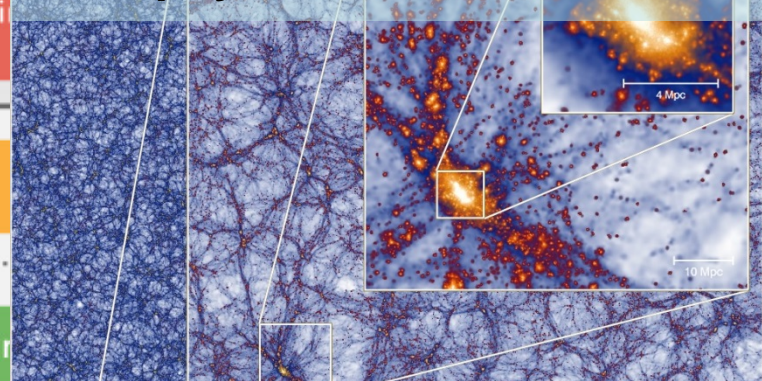
NSM Architecture

5 - 10 PF Systems

NKN Gigabit Link

100 -500 TF

100 -500 TF

5-10 PF Systems

10s TF

10s TF

NKN

10s TF

100 -500 TF

100 -500 TF

5 - 10 PF System

Supercomputing Systems & Applications are Challenging!

Application Layer	Meteorology	Petroleum	Aerospace	Animation	Life Science	...
Application Environment Layer	MPI	PVM	OpenMP	Math Library
Cluster Software Layer	CHESS Web Portal				
	CHESS System Deployment	CHESS Cluster Monitoring	CHESS Cluster Management	CHESS Job Scheduling	CHESS Reporting and Billing
System Software Layer	Linux OS	Compiler	Library
Hardware Layer	Server	Storage	Switch	Infrastructure

CHESS

Supercomputing Systems & Applications are Challenging!

Climate and Weather Modeling

Cosmic millennium -- Astrophysics

Reverse-Engineering the Brain
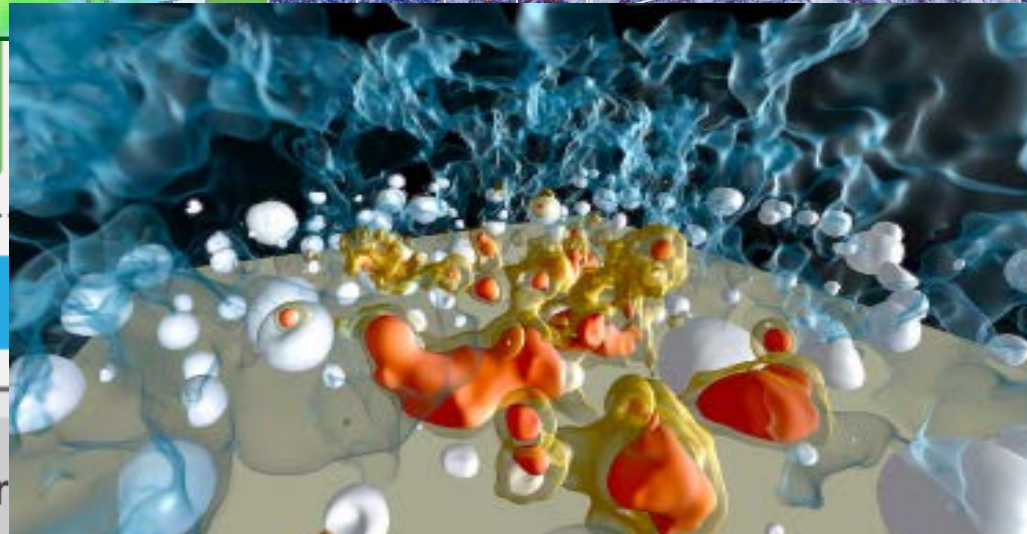
Computational Fluid Dynamics

Thank you !