Advanced Computational Testing and Simulation

BACKGROUND MATERIAL

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Motivation

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Grand Challenges are ..fundamental problems in science and engineering, with potentially broad social, political, and scientific impact, that could be advanced by applying high performance computer resources

Office of Science and Technology

- Some grand challenges: electronic structure of materials, turbulence, genome sequencing and structural biology, global climate modeling, speech and language studies, pharmaceutical design, pollution, etc. .

Motivation

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With the development of new kinds of equipment of greater capacity, and particularly of greater speed, it is almost certain that new methods will have to be developed in order to make the fullest use of this equipment. It is necessary not only to design machines for the mathematics, but also to develop a new mathematics for the machines - 1952, Hartree

- **Metropolis** grew out of physical chemistry in 1950's through attempts to calculate statistical properties of chemical reactions. Some areas of application: astrophysics, many areas engineering, and chemistry)
- **Fast Fourier Transform** (**FFT**): implementation of Fourier Analysis. Some areas of application: image and signal processing, seismology, physics, radiology, acoustics and engineering)
- **Multigrids**: method for solving a wide variety of PDE. Some areas of application: physics, biophysics and engineering

Motivation

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Computational science: can be characterized by the needs to gain understanding through the analysis of mathematical models using high performing performing computers

Community
- Scientists
- Engineers
- Mathematicians
- Economists, artists

Multidisciplinary!

Computer Science	Mathematics:
Provides services ranging from Networking and visualization tools to algorithms	credibility of algorithms (error analysis, exact solutions, expansions, uniqueness proofs and theorems)

Motivation - Example I

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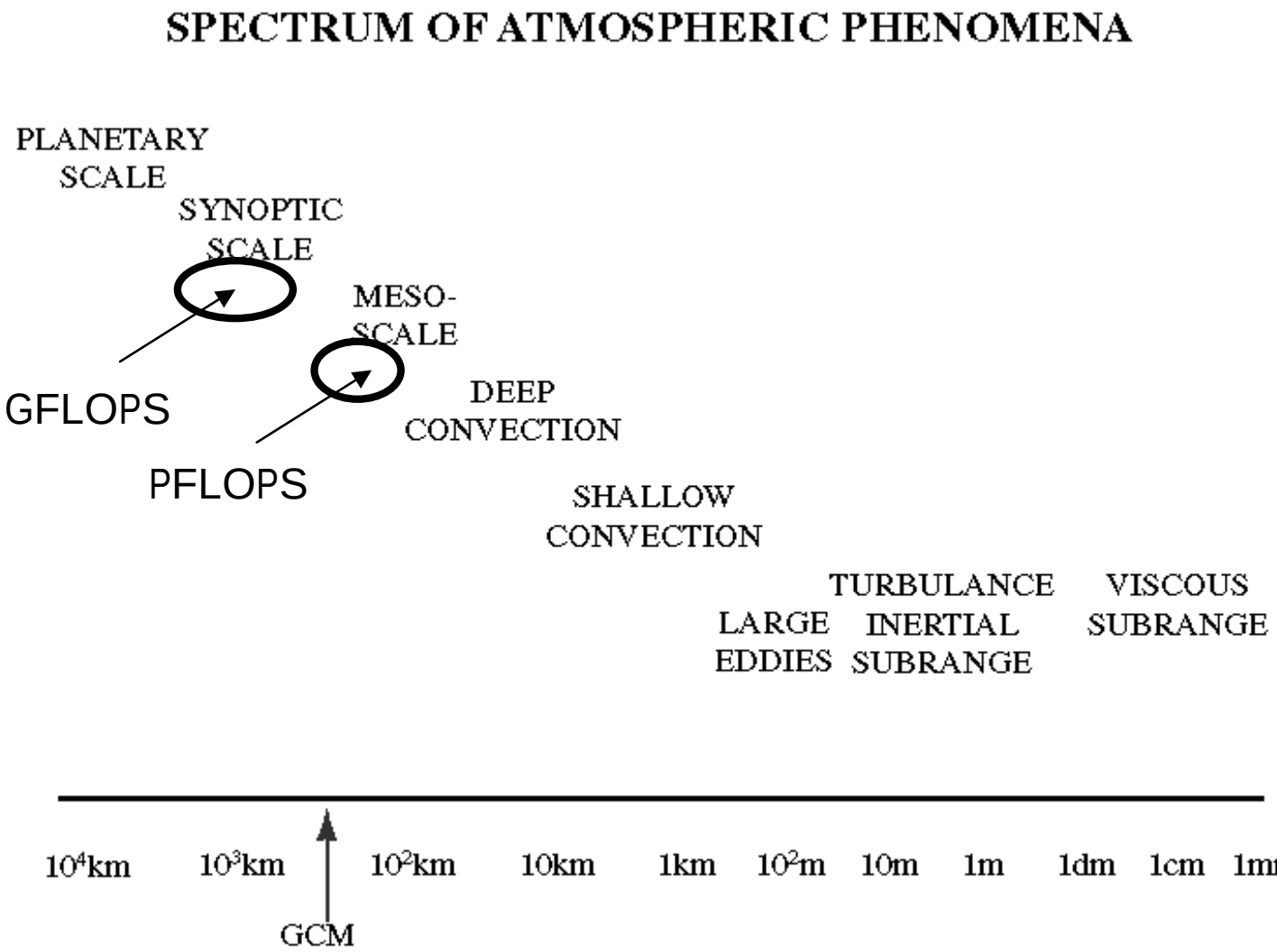

Motivation - Example II

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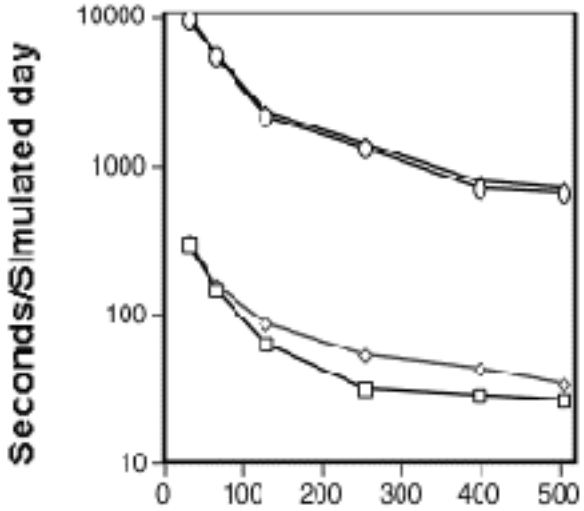
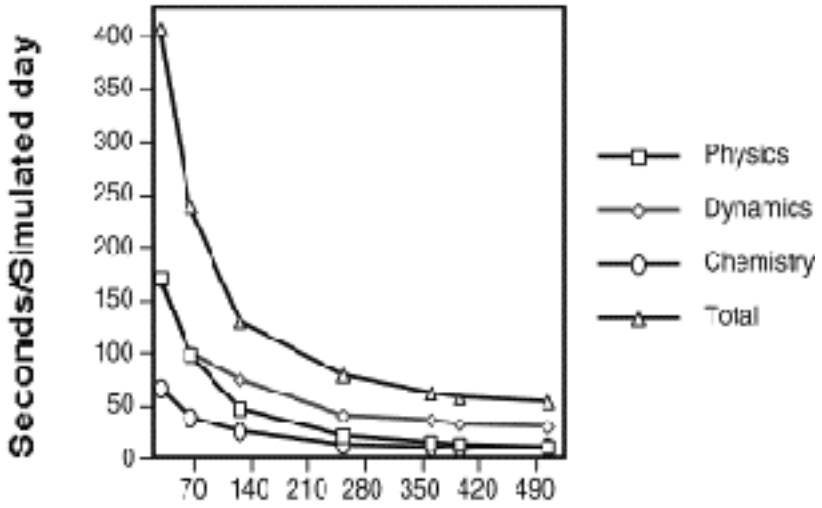


AGCM/ACM
2.5 long x 2 lat, 30 layers
25-chemical species



AGCM/ACM
2.5 long x 2 lat, 30 layers
2-chemical species

- **Non-linear demand for resources (CPU - Memory)**
- **Multi-disciplinary application is more demanding**

The Hardware

Flynn's Taxonomy

	Single Data Stream	Multiple Data Stream
Single Instruction Stream	**SISD**	**SIMD**
Multiple Instruction Stream	**MISD**	**MIMD**

High Performance Computers

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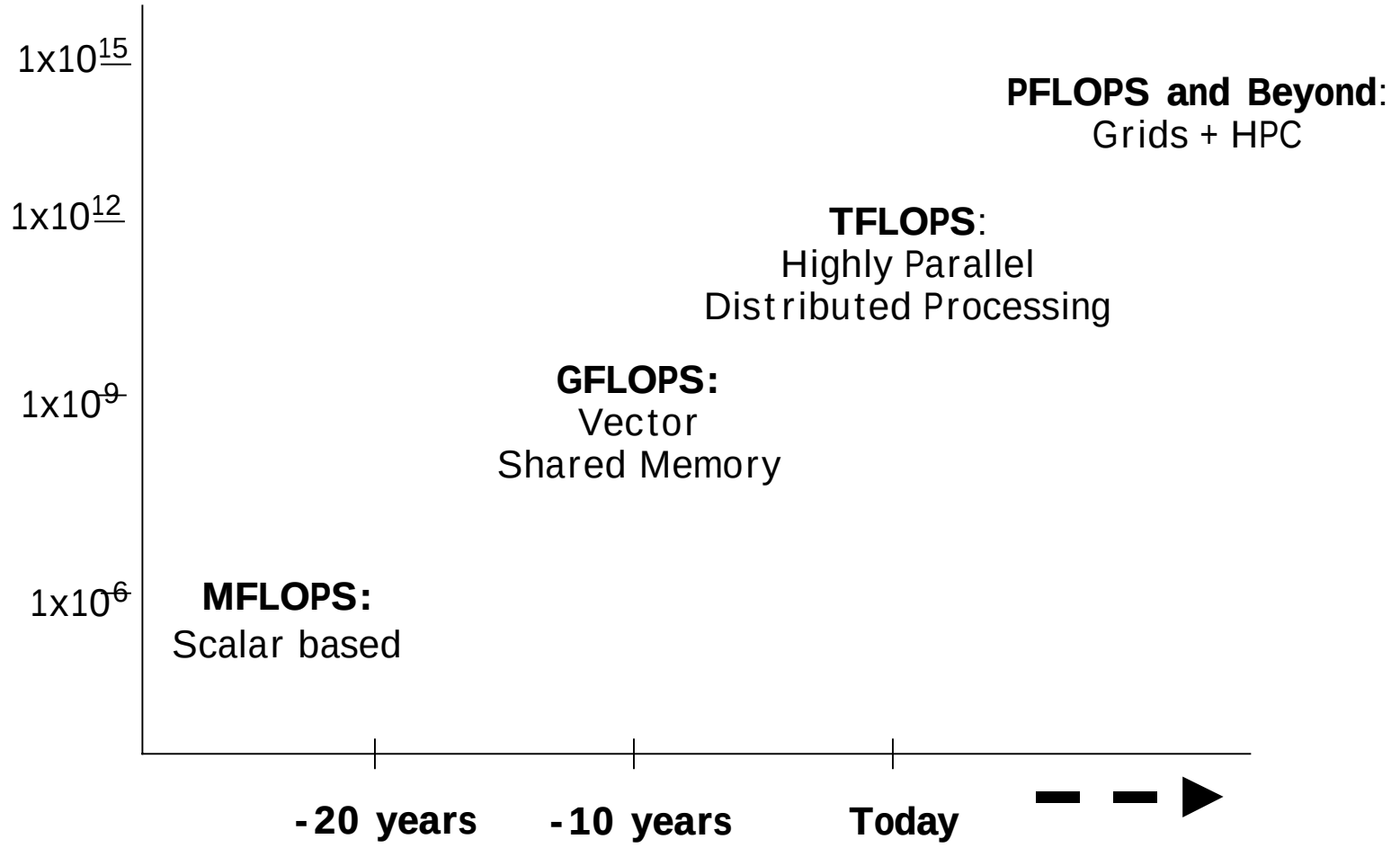
FLoating **P**oint **O**perations/**S**econd (**FLOPS**)



The GRID

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- A large pool of resources
  - Computers
  - Networks
  - Software
  - Databases
  - Instruments
  - people

Requirements from GRID implementation:

- Ubiquitous: ability to interface to the grid at any point and leverage whatever is available
- Resource Aware: manage heterogeneity of resources
- Adaptive: tailored to obtain maximum performance from resources

Shared vs. Distributed Memory

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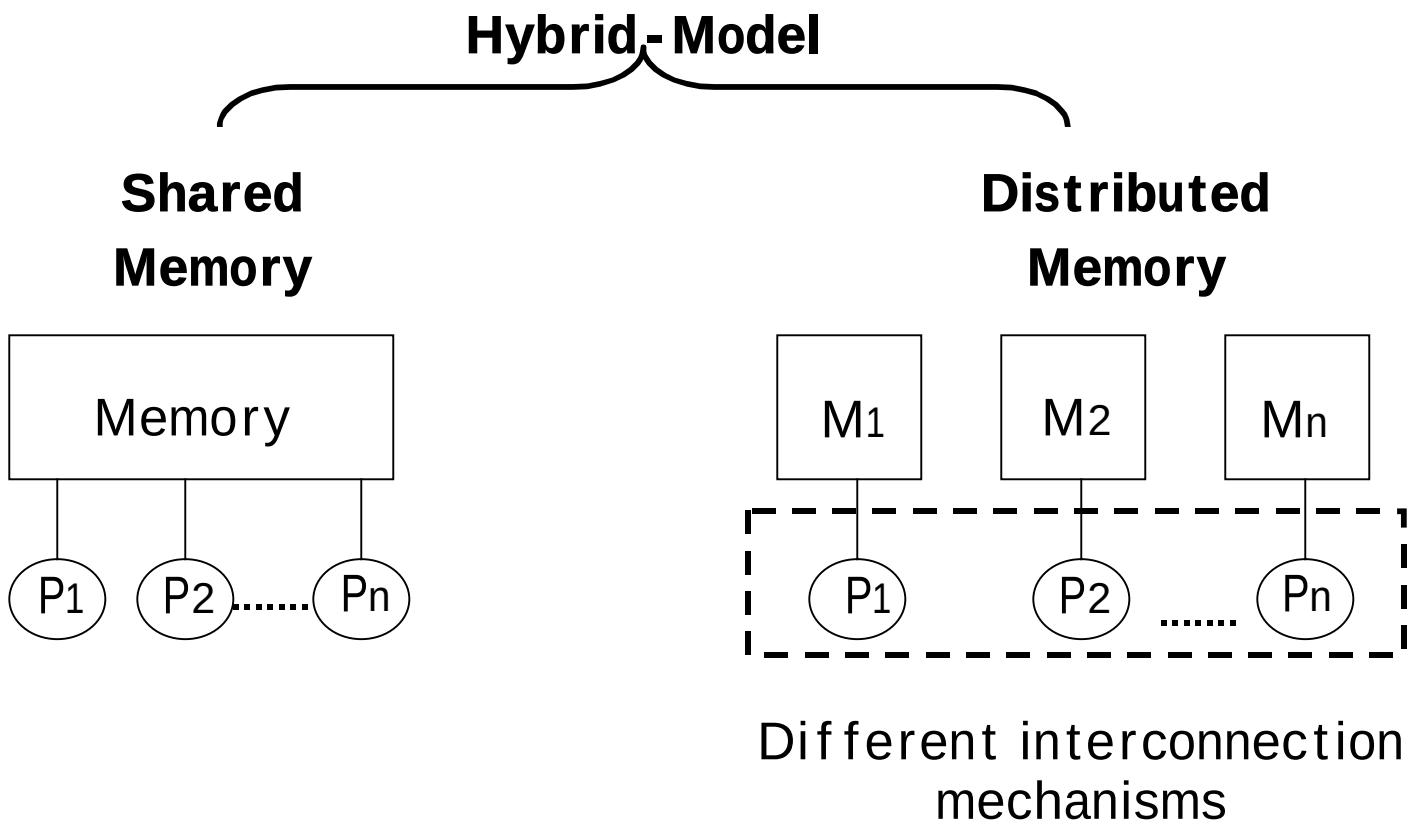

Different interconnection mechanisms

Memory Hierarchy

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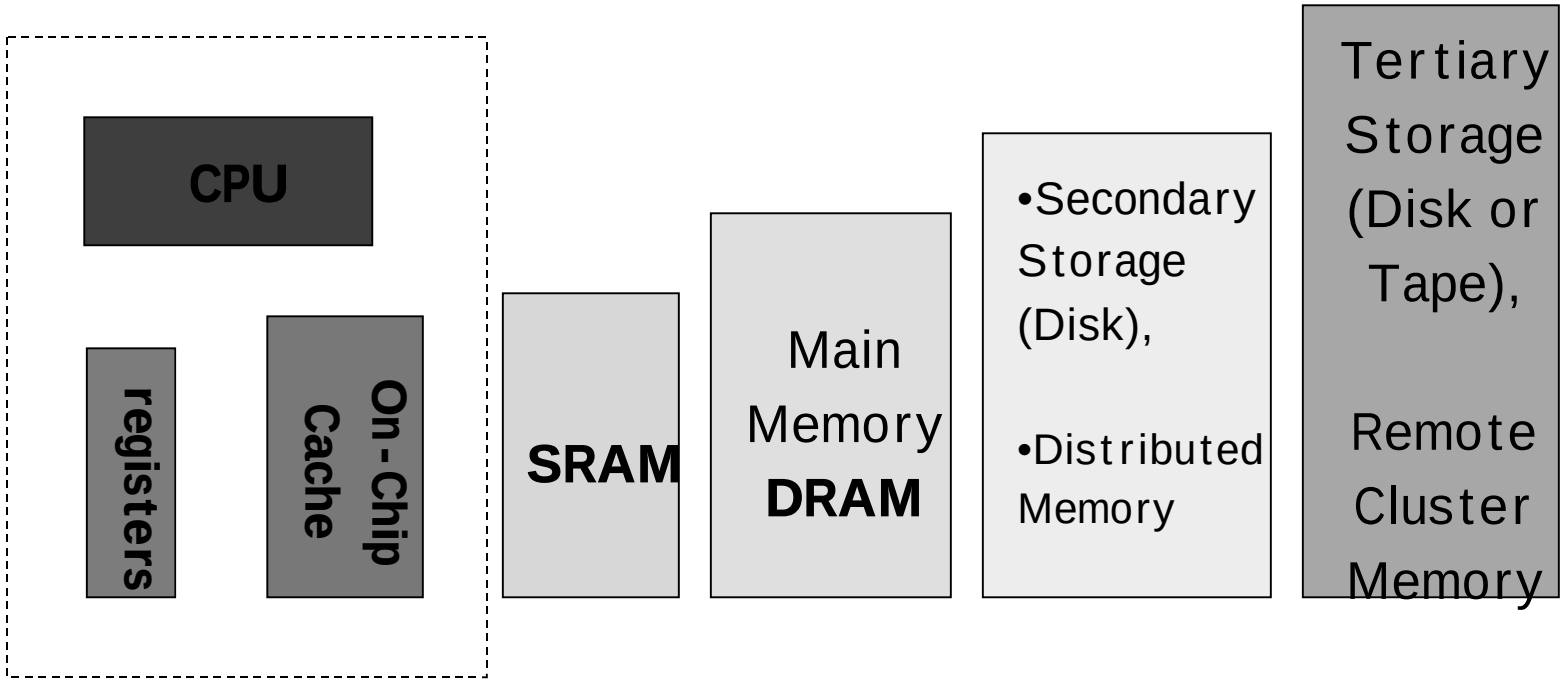
- *Where is the data? Why is data locality important?*



Speed	1's ns	10's ns	100's ns	.1's -10's ms	10's s
Size	100's bytes	Kbytes	Mbytes	Gbytes	Tbytes

Using the hardware

Levels of Parallelism

- Job and Task Level : Highest level of parallelism. Multidisciplinary applications running on a single computational resource or a collection of heterogeneous ones.

- Program Level: A single program and/or data is broken down into constituent parts

- Instruction Level: Pipeline and data streams

- Arithmetic and bit Level: Lowest level- CPU level

Parallel Programming Paradigms

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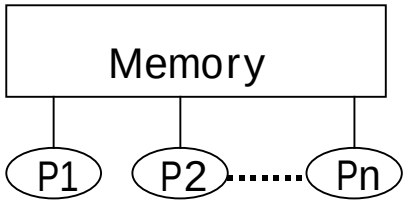
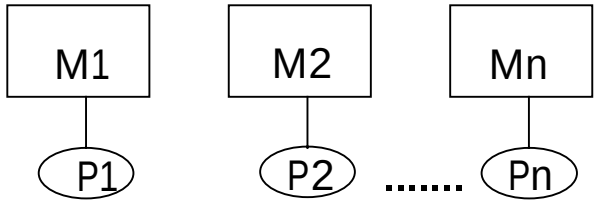
Shared Memory



- Data parallelism
- easier to implement
- shared memory space
- mutual exclusion, contention

- Message Passing
- shared area is use for sending and receiving data

Distributed Memory



- virtual shared memory
- data is implicitly available to all

- Implicit mutual exclusion
- Only explicit synch
- Depends on Memory Hierarchy and Network

CPU vs. DRAM Performance

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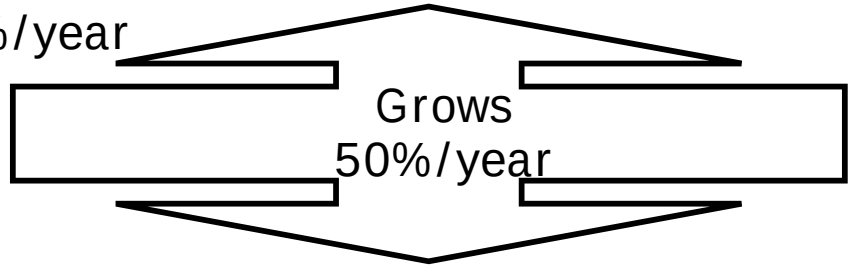
• Since 1980's, µProcs performance has increased at a rate of almost 60%/year



• Since 1980's, DRAM (latency) has improved at a rate of almost 9%/year

•Software required to bridge this gap

- Tuned or optimized to existing hardware capabilities
- Handle user needs (computational sciences)
- Portable + Interoperable

ACTS Tools Categorization

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- Numerical
  - software that implements numerical algorithms
- Support for Code Development
  - software that manages data, communication
- Support for Code Execution
  - runtime, support tools, developer's bag
- Library Optimization
  - Tuning for library and compiler development
- Interoperability
  - Library, Language and component

Some Numerical Tools

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- **Trilinos**: iterative methods for solving sparse linear systems **M. Heroux**
- **Hypre**: collection of advanced preconditioners **Yang**
- **PETSc**: methods for the solution of PDE related problems **Balay and Curfman-McInnes**
- **PVODE**: is a solver for large systems of ordinary differential equations on parallel machines. **Hindmarsh**
- **ScaLAPACK**: dense linear algebra computations **Marques**
- **SuperLU**: direct methods for sparse linear systems **Li**
- **TAO:** Toolkit for Advanced optimization **Moré and Benson**

Tools for Code Development

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- **Global Arrays**: portable, distributed array library, shared memory style of programming **Tipparaju**
- **Overture**: library of grid functions which derives from P++ arrays **Quinlan**

Tools for Code Execution Support

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- **CUMULVS** (Collaborative User Migration User Library for Visualization and Steering) **Kohl**
- **Globus**: infrastructure for high performance distributed computing. Bag of services for the grid **Heahey**
- **PAWS** (Parallel Application WorkSpace) provides interapplication support in heterogeneous computing environments **Sottile**
- **SILOON** (Scripting Interface Languages for Object-Oriented Numerics): scripting features **Sottile**
- **TAU** (Tuning and Analysis Utilities): advanced performance analysis and tuning **Shende**

Frameworks
Scientific Computing and Programming

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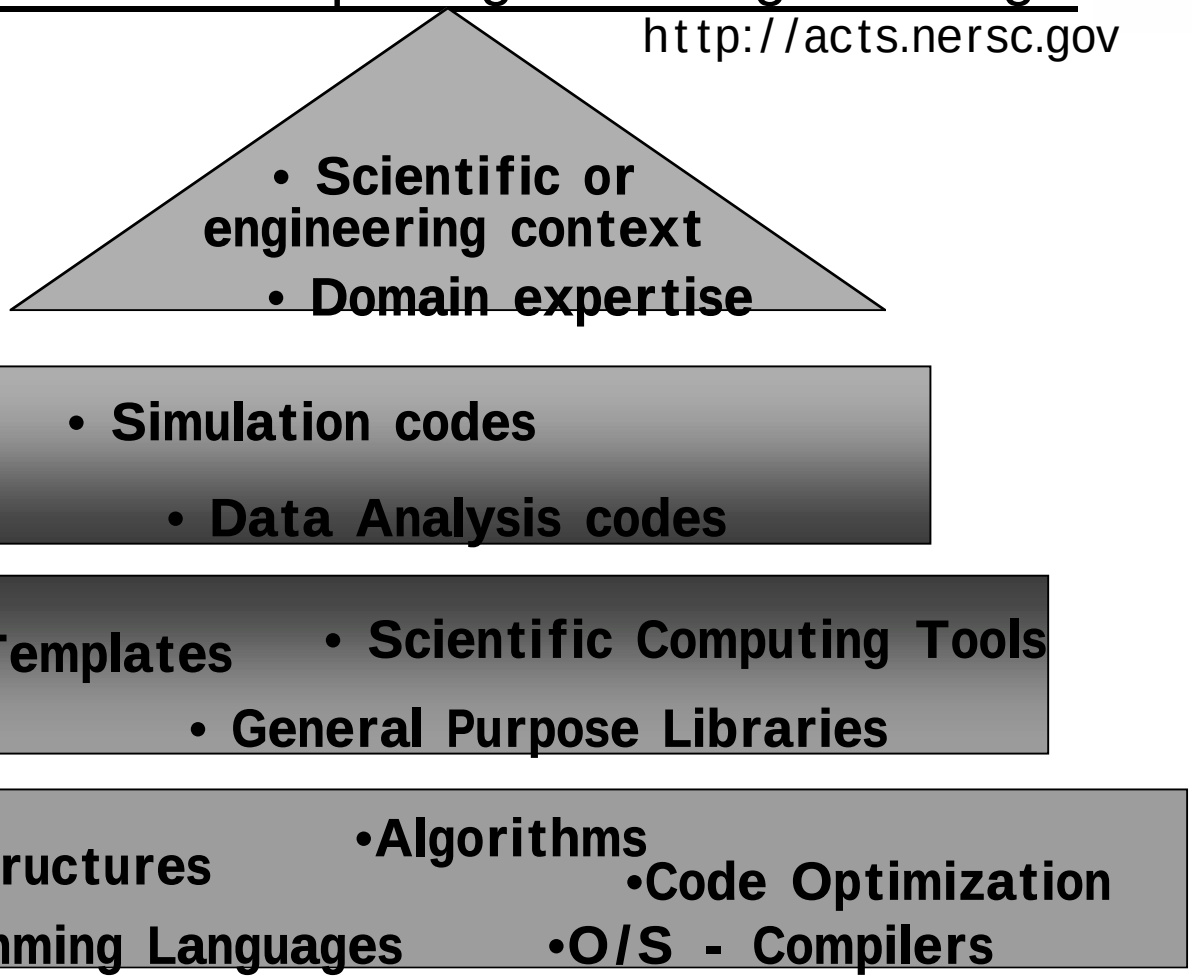

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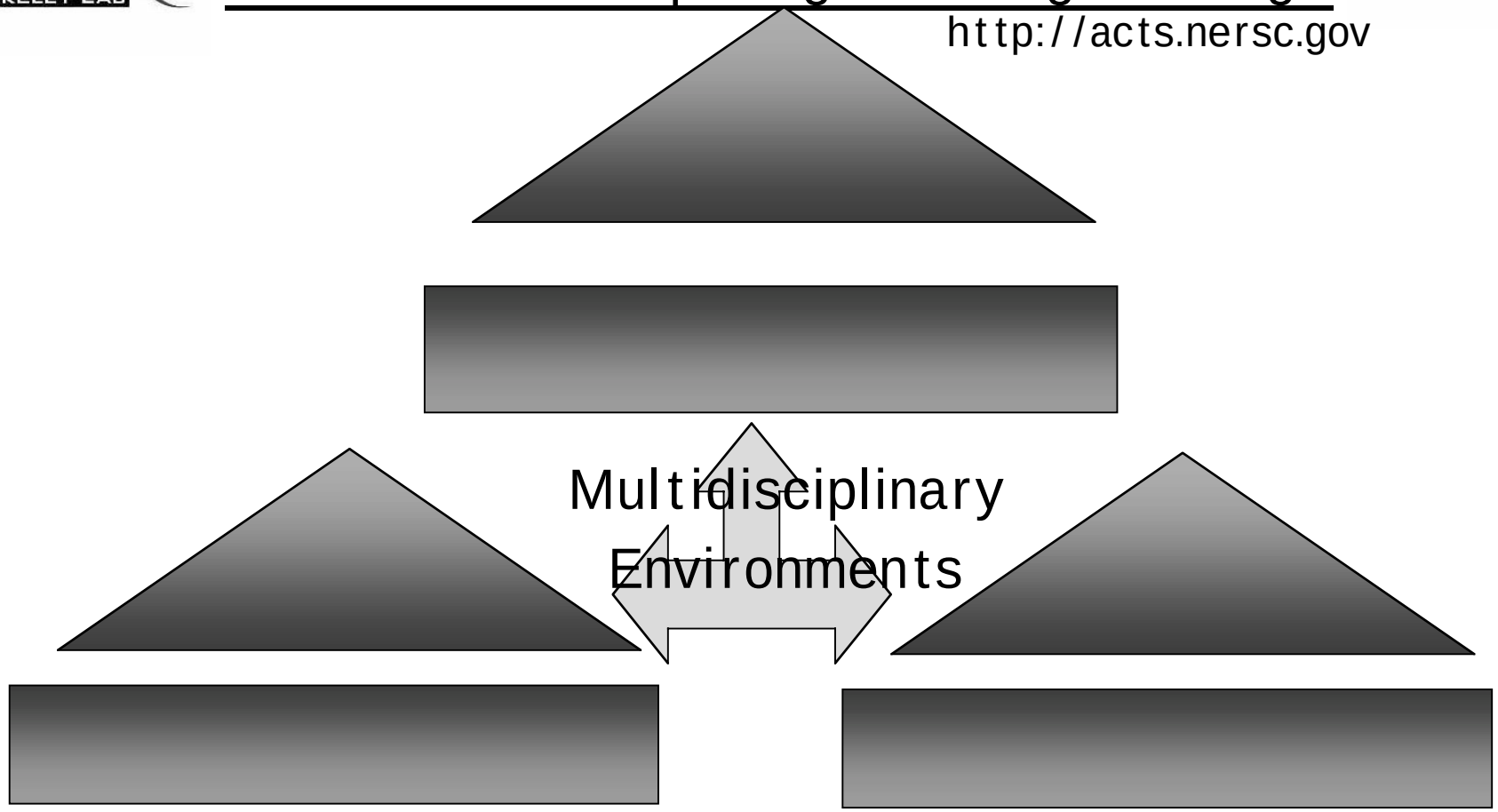

Hardware - Middleware - Firmware

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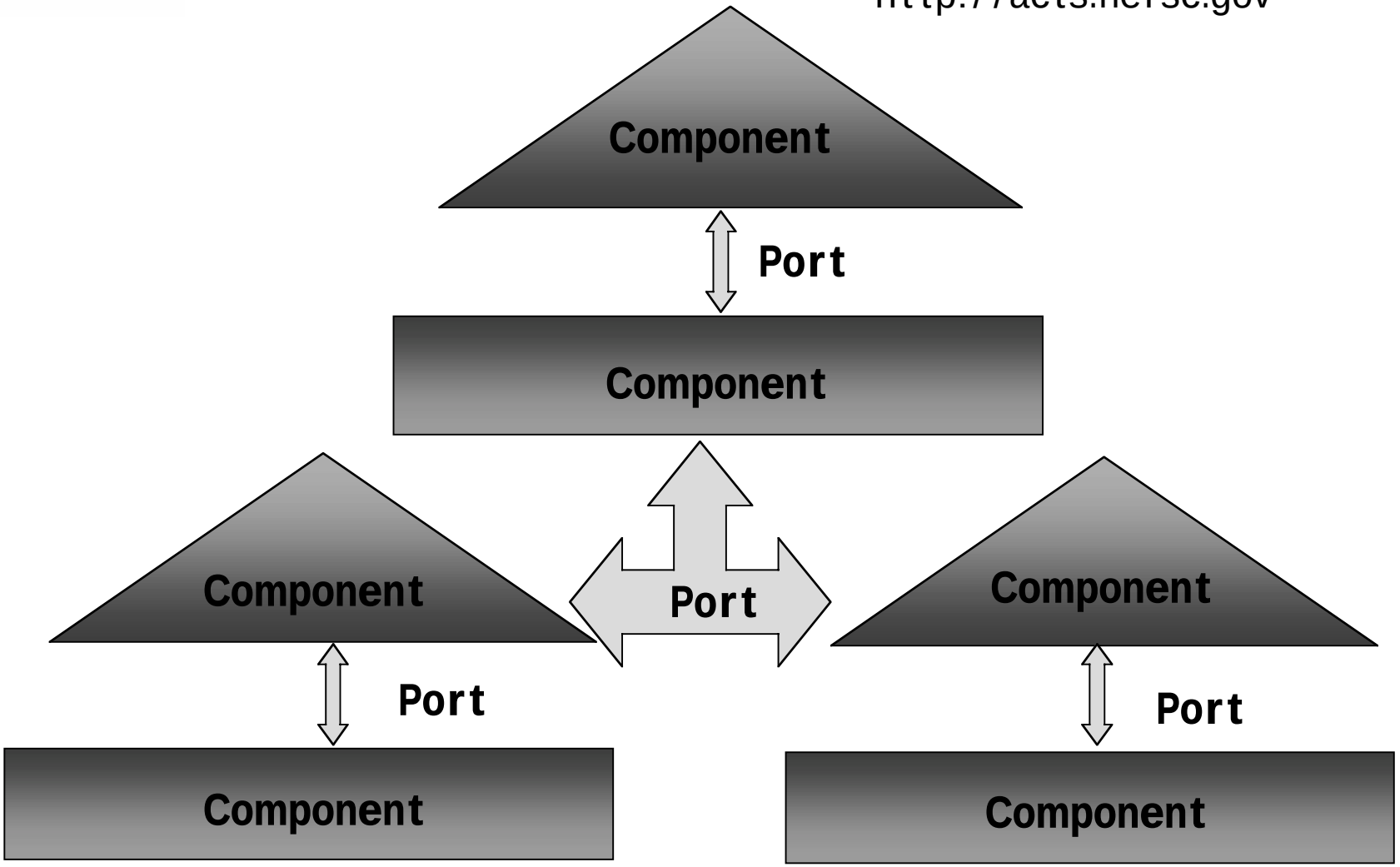

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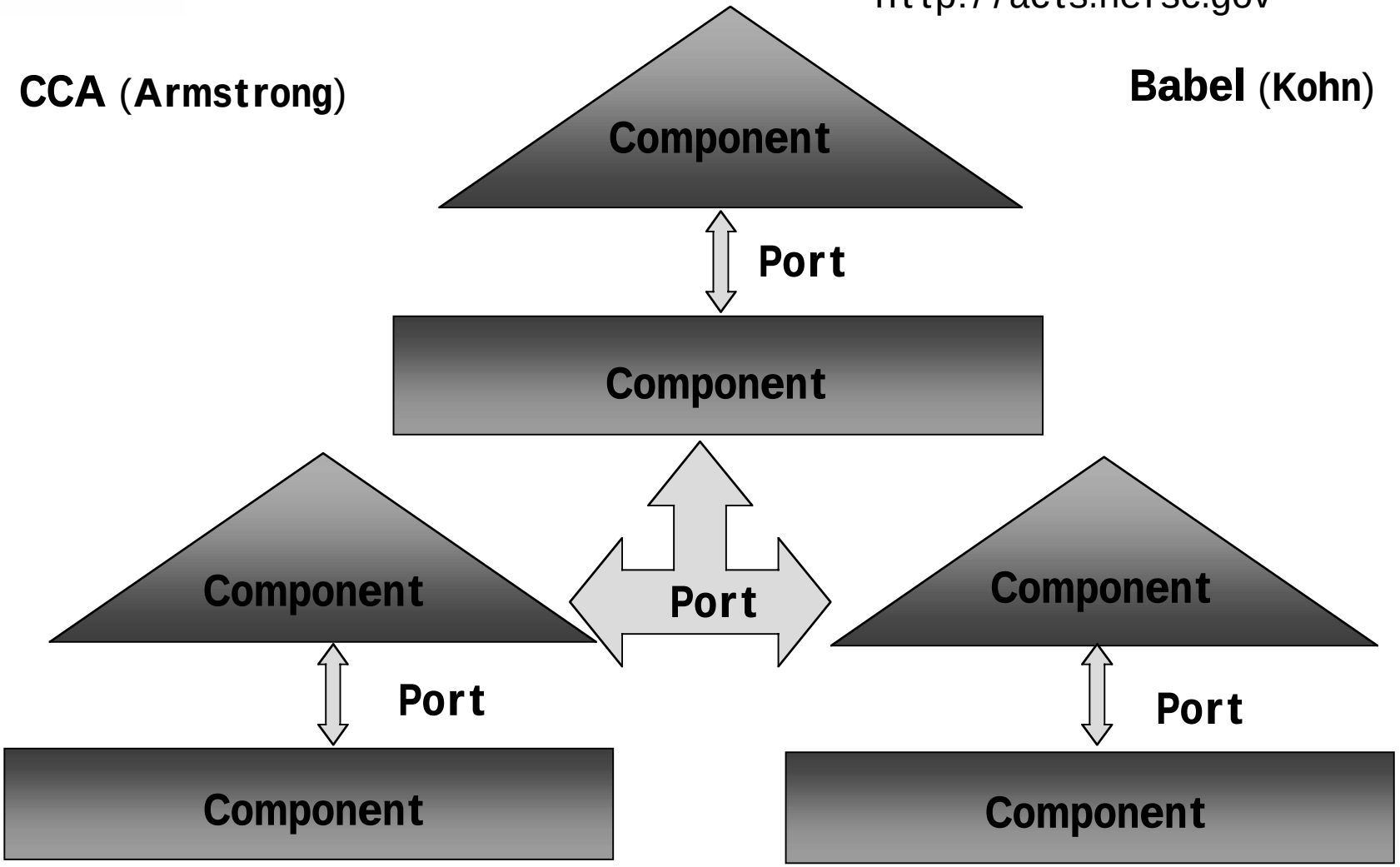
CCA (Armstrong)

Babel (Kohn)



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