Beyond the Desktop

- The role of computational architectures in accelerating discovery
- Mohammed Khaleel, Ph.D.

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Outline

- High-performance computing systems
  - *Beyond the Desktop*
- Traditional (or “mainstream”) supercomputers
  - Science applications
- Multithreaded supercomputers
  - Cybersecurity applications
- Energy Efficiency
- Back to the Desktop

High-Performance Computing Systems

- Nowadays, HPC systems are *parallel* computing systems
  - Consisting of hundreds of processors (or more)
  - Connected by high bandwidth, low-latency networks
    - Collections of PCs connected by Ethernet *are not* HPC systems
  - Basic building block is a *node*: server-like computer (a few processor sockets, memory and network interconnect cards, possibly I/O devices).
- Nodes are parallel computers on their own: contain usually >= 2 processor sockets with multiple cores per processor
  - Looks very similar to what you have on your desktop PC!!
- HPC systems have a multiplicity of applications in scientific and engineering areas: physics, chemistry, biology, material design, mechanical design.

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HPC Systems (cont.)

- Two basic kinds of HPC systems:
  - Distributed memory systems
  - Shared memory systems
- Distributed memory HPC systems:
  - Typical HPC system, processors only have direct access to local memory on the node.
  - Remote memory on other nodes must be accessed indirectly via a library call.
  - Can scale to tens and hundreds of thousands of processors (Blue Gene/P @ LLNL, Chinook @ EMSL/PNNL)
- Shared memory HPC systems:
  - Processors have *direct* access to local memory on the node *and* to remote memory on other nodes.
  - Speed of access may vary
  - More difficult to scale beyond a few thousand processors (Columbia SGI Altix @ NASA)

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Chinook (supercomputer at EMSL/PNNL)

- 2310 node HP cluster
  - Dual quad-core processors per node
  - Total: 18,480 cores

Feature	Detail
Interconnect	DDR InfiniBand (Voltaire, Mellanox)
Node	Dual Quad-core AMD Opteron 16 GB memory
Local Scratch	400 MB/s, 924GB/s aggregate 440 GB per node. 1 PB aggregate
Global Scratch	30 GB/s 250 TB total
User /home	1 GB/s 20 TB total

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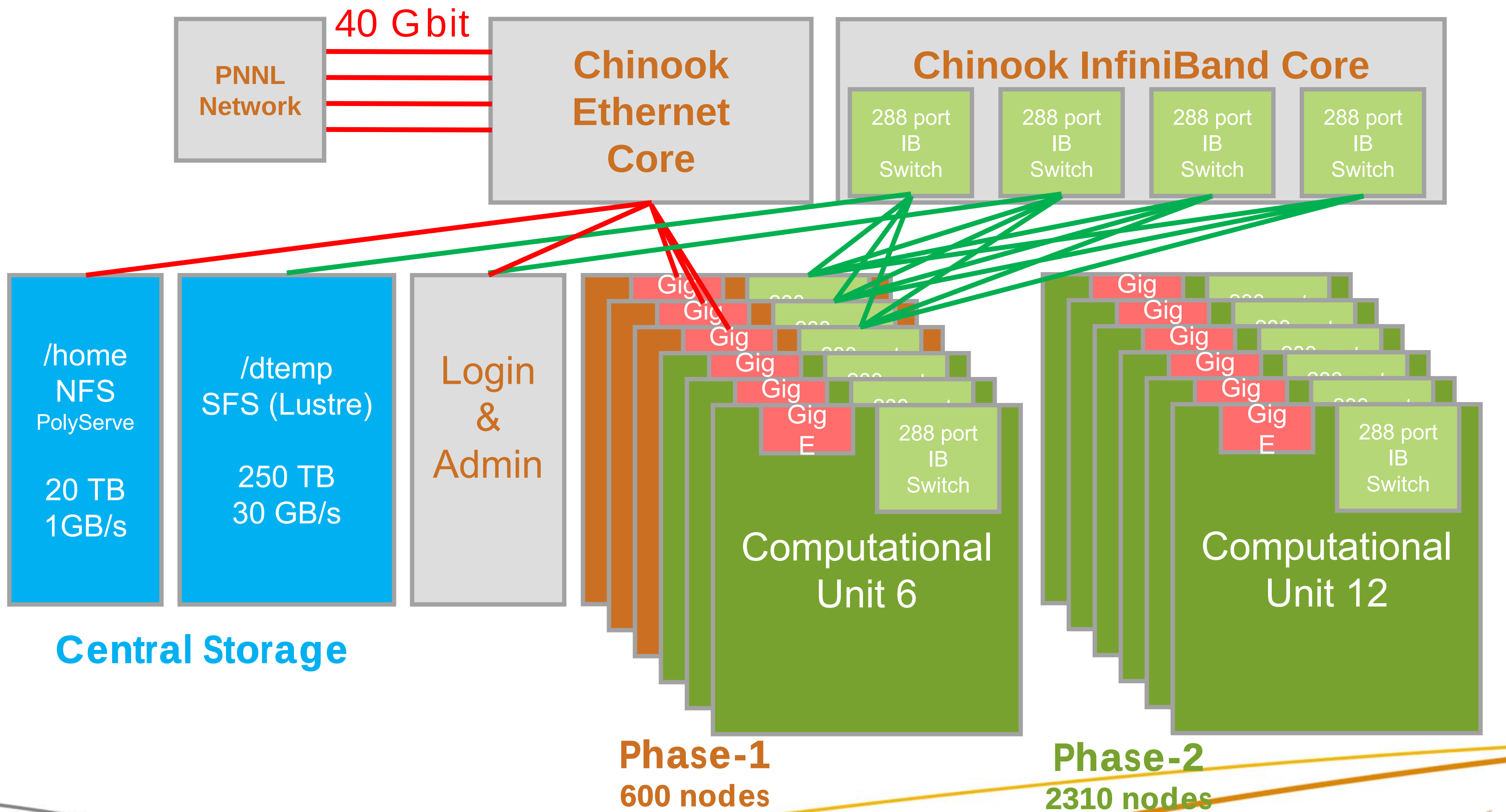
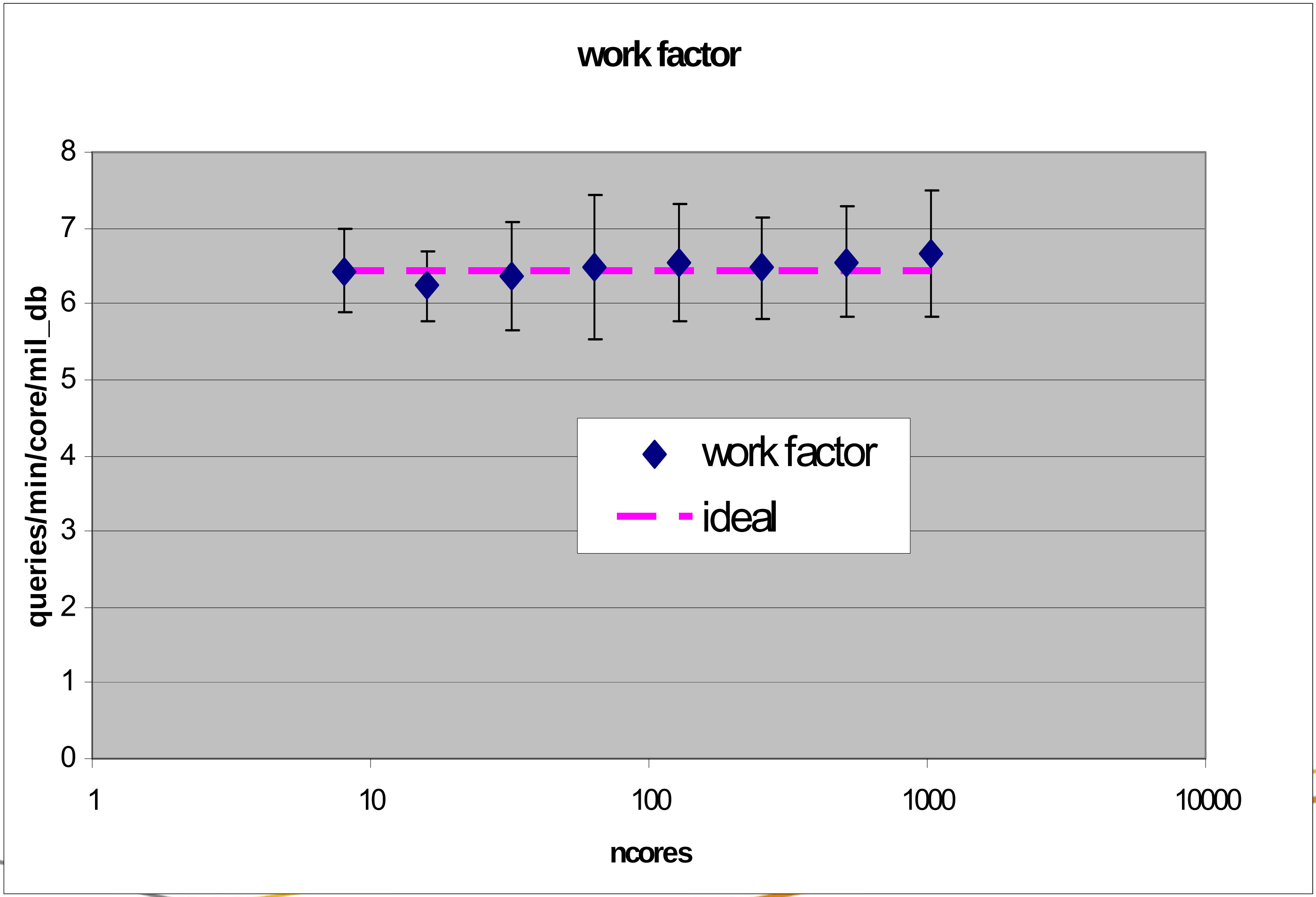
Chinook cluster architecture



Chinook software scalability

- ScalaBLAST scalability plot



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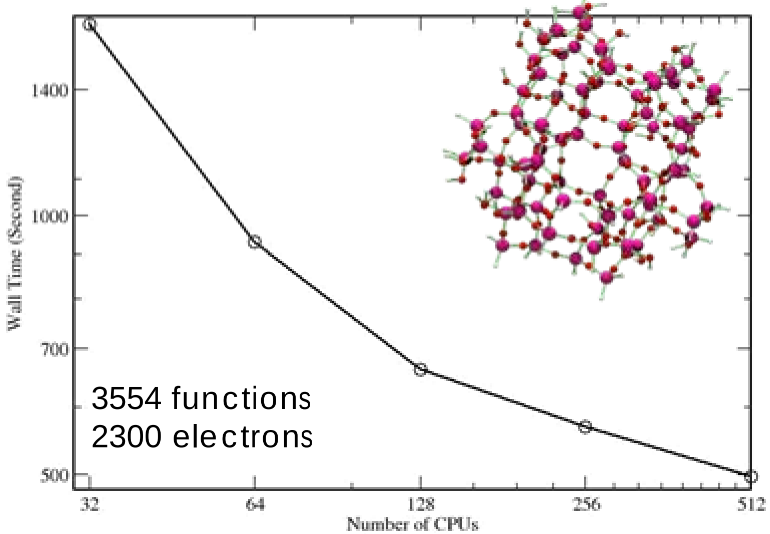
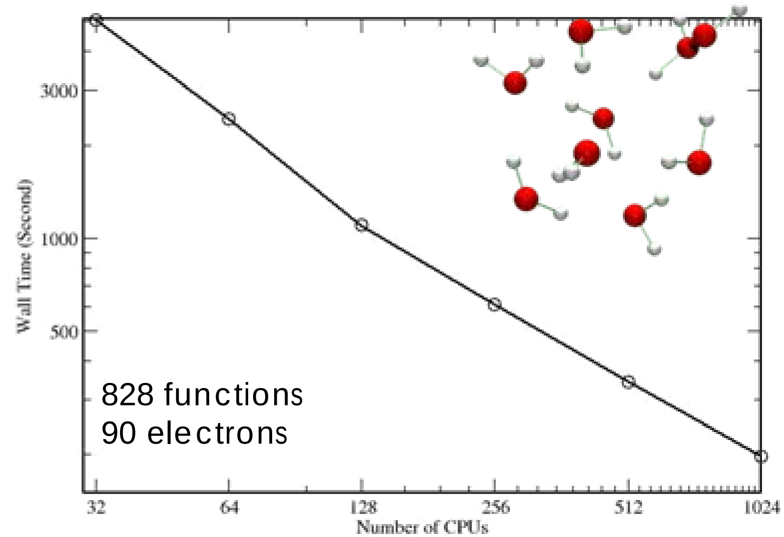
NWChem on Chinook (log-log plots)

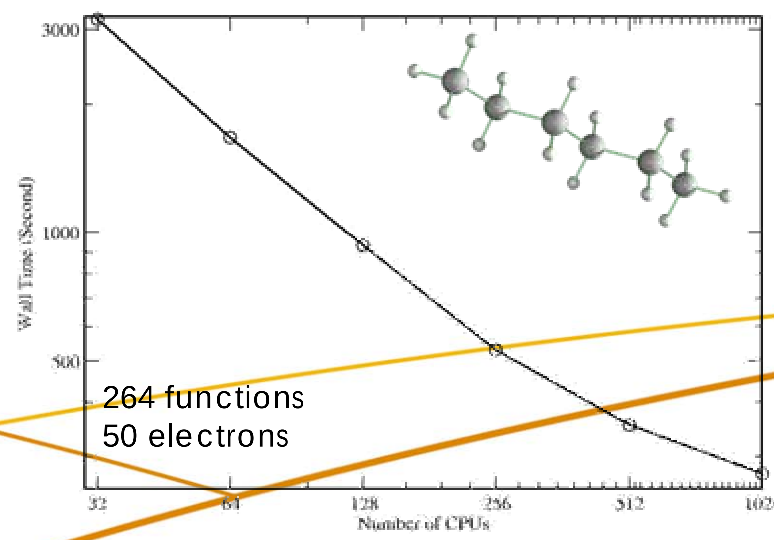
$Si_{75}O_{148}H_{66}$ with DFT



$(H_2O)_9$ with MP2



C_6H_{14} with CCSD(T)



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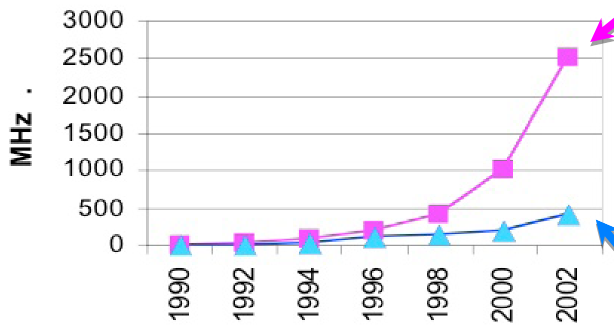
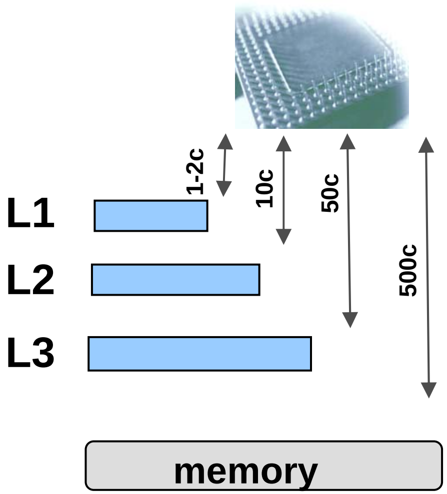
Processor Architecture (cont.)

Processor speed





Memory speed

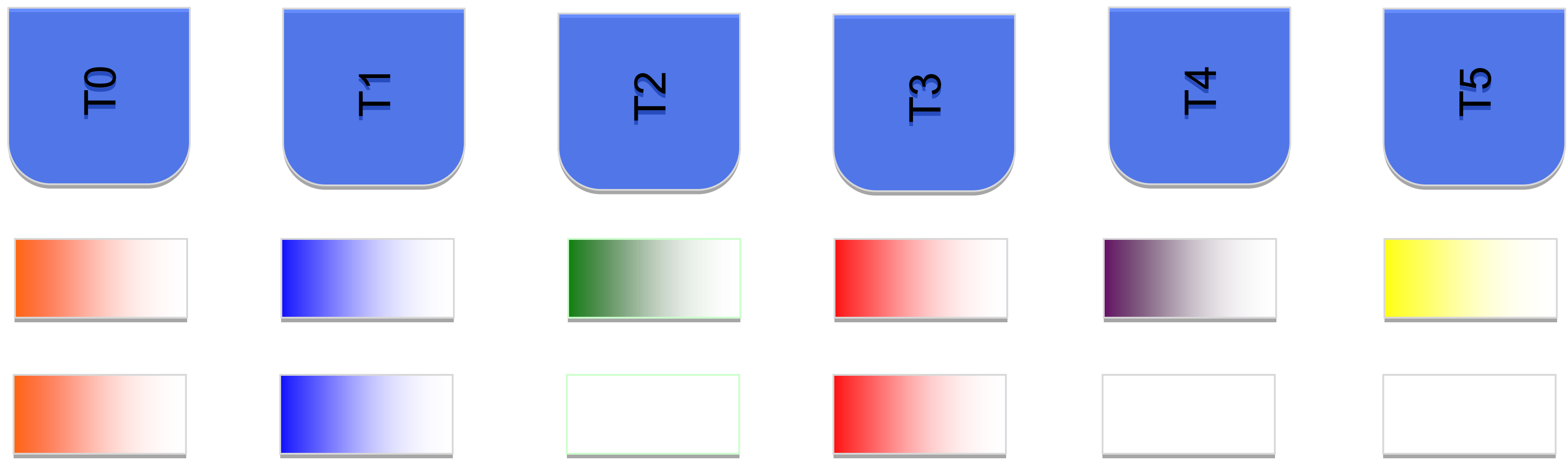
W. Wulf S. McKee, “Hitting the memory wall: Implications of the obvious”, ACM Computer Architecture News, 1995

Memory Wall Problem

Multithreaded Processors

- Commodity memory is slow, custom memory is very expensive:
  - What can be done about it?
- Idea: cover *latency* of memory loads with other (useful) computation
  - OK, how do we do this?
- Use multiple execution contexts on the same processor, switch between them when issuing load operations
  - Execution contexts correspond to threads
- Examples: Cray ThreadStorm processors, Sun Niagara 1 & 2 processors, Intel Hyperthreading

Multithreaded Processors (cont.)



Each thread has its own independent instruction stream (program counter)

Each thread has its own independent register set

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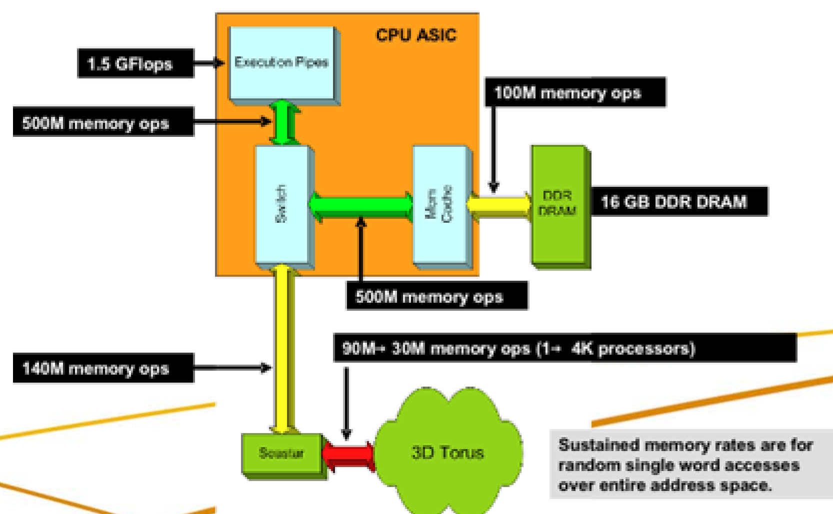
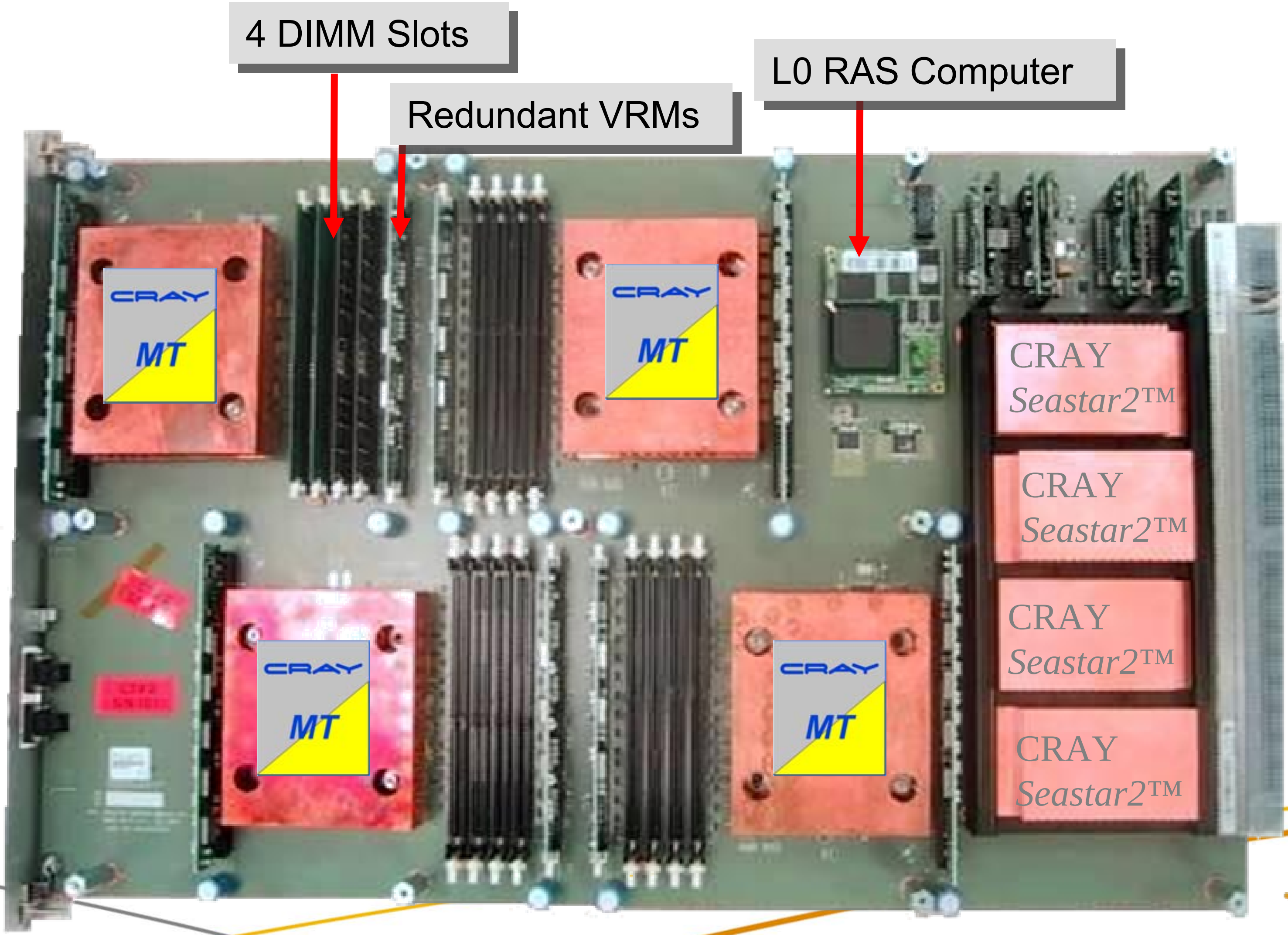
Cray XMT multithreaded system

- ThreadStorm processors run at 500 MHz
  - 128 hardware thread contexts, each with its own set of 32 registers
  - ***No*** data cache
  - 128KB, 4-way associative data buffer on the *memory side*
  - Extra bits in each 64-bit memory word: full/empty for synchronization
  - Hashed memory at a 64-byte level, i.e. contiguous logical addresses at a 64-byte boundary are mapped to uncontiguous physical locations
- Global shared memory
- Scalable to 8,192 processors

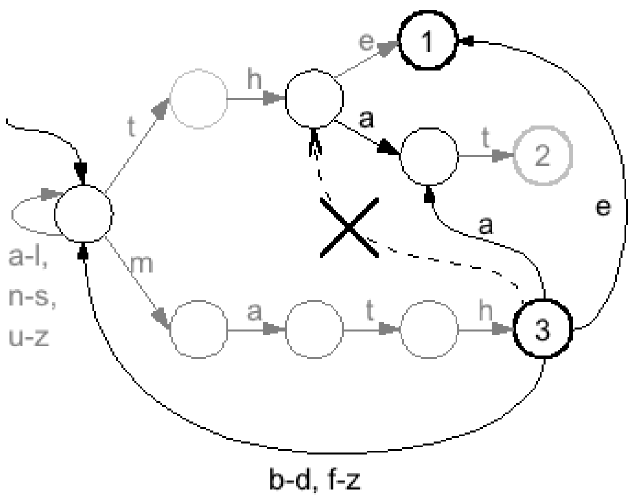


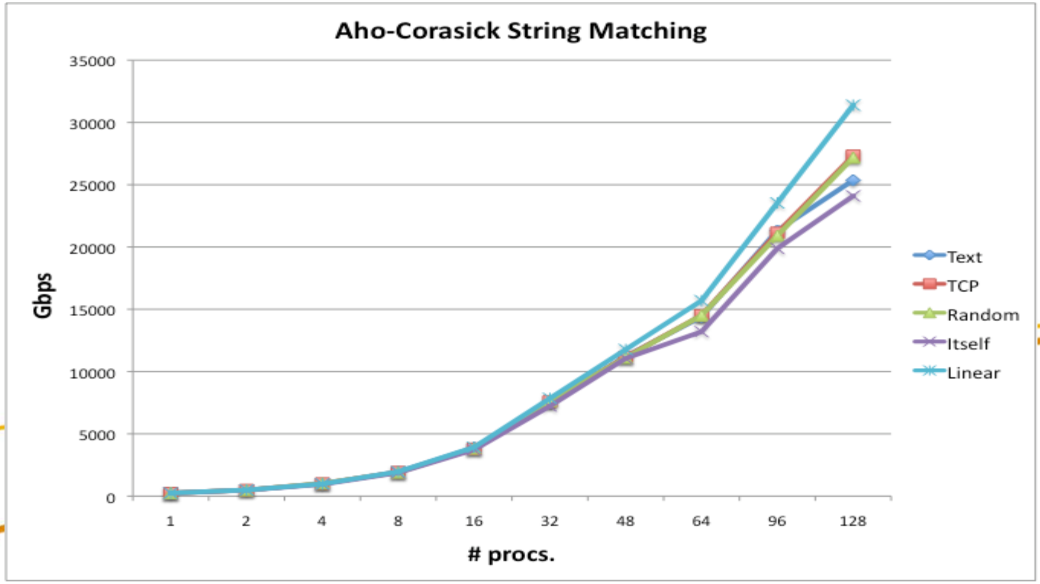
Cray XMT multithreaded system (cont.)



High-Performance String Matching on the Cray XMT

- Fast, scalable string matching is at the base of modern cybersecurity applications
  - Deep packet inspection for malware
- Performance has to be consistent and content independent
  - At the same system should be flexible and programmable
  - Prevent content-based attacks
- Excellent scalability and performance on the XMT





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EPA reports energy used in U.S.

- ~ 61 billion kilowatt-hours (kWh) in 2006
- 1.5% of total electricity consumption
- Total electricity cost of about $4.5 billion.
- Similar to the amount of electricity consumed by approximately 5.8 million average U.S. households (or about five percent of the total housing stock).
- Federal servers and data centers alone
  - ~ 6 billion kWh
  - 10% of electricity used for servers and data centers
  - Total electricity cost of about $450 million annually.

EPA Report to Congress on Server and Data Center Energy Efficiency **R**eleased On August 2, 2007 and in response to Public Law 109-431

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Current Power Usage by Chinook, MSCF System at PNNL

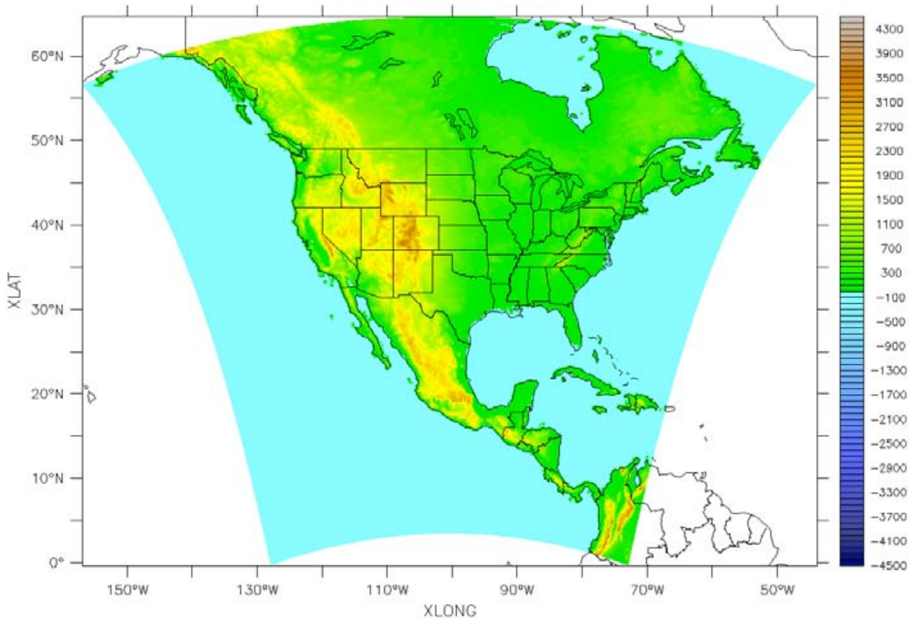
- Chinook (160TF peak), has 2310 dual socket quad-core AMD Opteron (2.2GHz) based servers from HP each with 16 GB memory, 365 GB local disk, a DDR Infiniband interconnect, and 297 TB global disk
- Consumes nearly 1.9 MW
  - ~ 1/3 for cooling
  - ~ 2/3 compute power (1.25 MW)
    - 40% of compute power is lost to power delivery (rectifier, UPS, Feed, PDU, power supply, voltage regulator)
- Average power efficiency for HPL
  - no losses: 133MFlop/s/W
  - with power delivery losses: 80MFlop/s/W
  - with power- and cooling delivery losses: 52MFlop/s/W

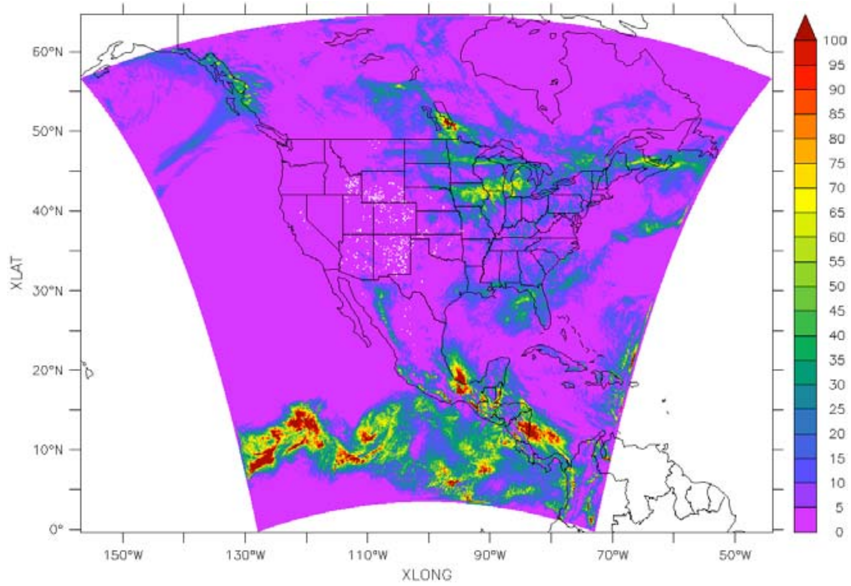
Compute Power

40% of compute power lost in power delivery

Top500 measures here

Regional Weather Forecasting (WRF)





Multiple concurrent basic 4.5 days weather forecasts for North&Central America

- Initialization: 1° Global Forecast System analysis from National Weather Service
- Decomposition: 480x480 cartesian grid (15km) with 45 levels
- Solver: Horizontal: Explicit High-Order Runge-Kutta; Vertical: Implicit
- Output: asynchronous 2.3GB netCDF every 3 model-hours per forecast

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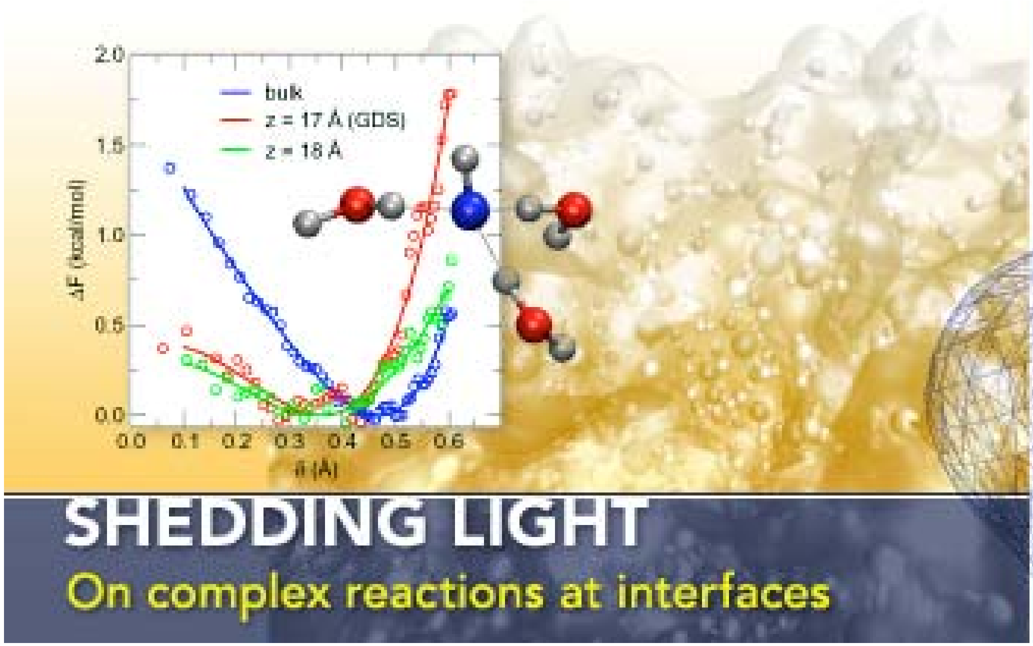
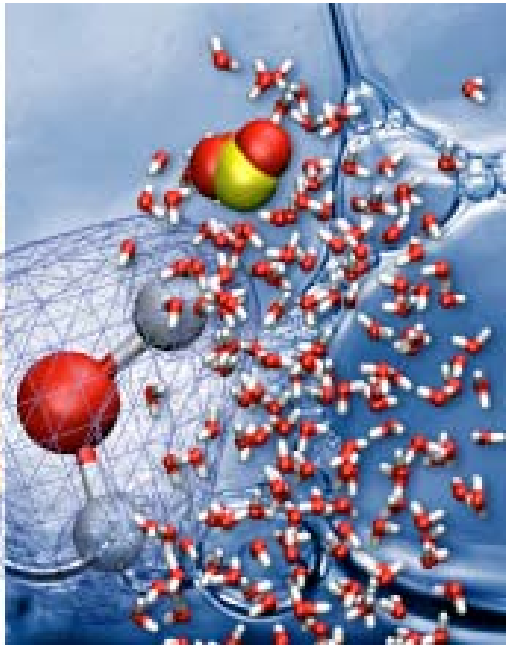
QM Computational Chemistry (CP2K)





Multiple concurrent liquid-vapor interface model simulations

- Initialization: Standard slab geometry (15x15x71Å^3)
- Decomposition:; 215 H_2O with single hydroxide ion
- Solver: Density Functional Theory with dual basis set (Gaussian & Plane-Wave)
  in conjunction with molecular dynamics and umbrella sampling
- Output: synchronous 75MB per 20k 0.5fs model-steps (MD time step)

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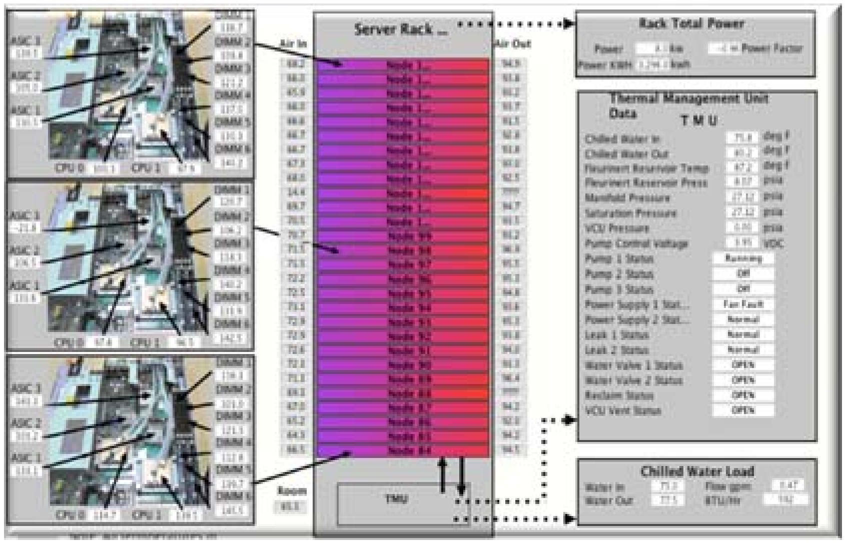
Device Under Test: NW-Ice

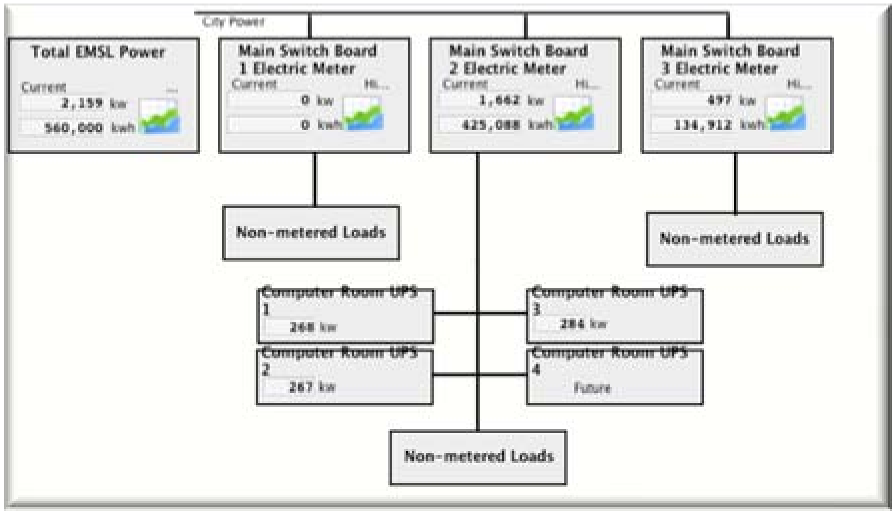
- 192 servers, 2.3 GHz Intel (quad-core) Clovertown, 16 GB DDR2 FBDIMM memory,160 GB SATA local scratch, DDR2 Infiniband NIC
- Five racks with evaporative cooling at processors
- Two racks air cooled
- Lustre Global File System
  - 34TB mounted
  - 49TB provisioned

Contributors to Power Consumption: Power Distribution



Facility:

- Transformers
- Rectifiers
- UPS
- Inverters



Data Center:

- Power Distribution Units
- Power Supply Units
- Voltage Regulators

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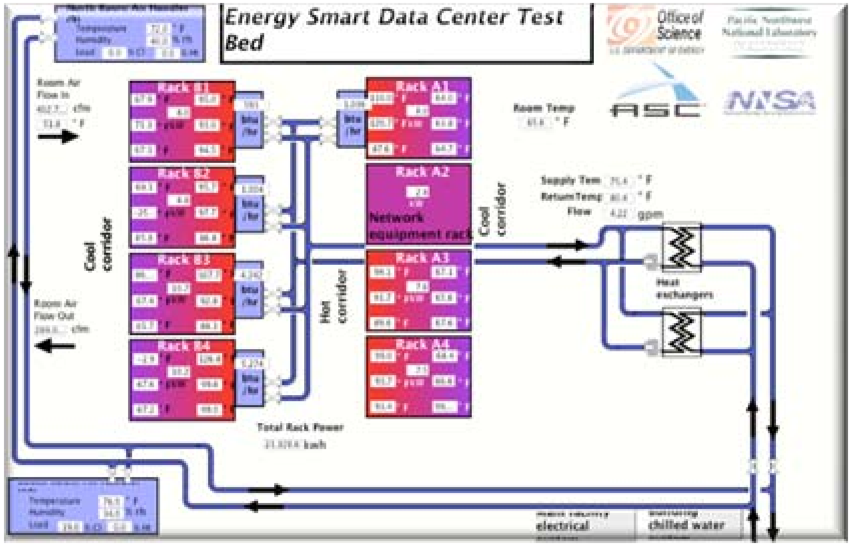
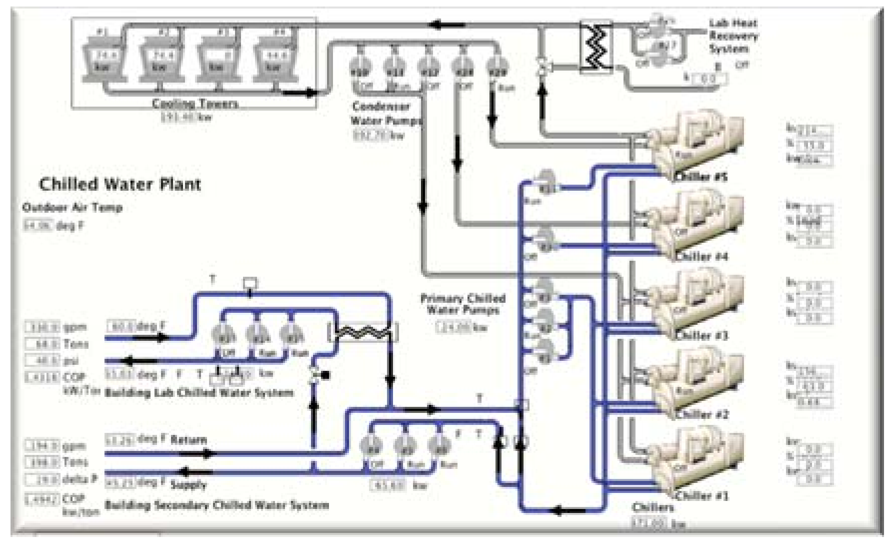
Contributors to Power Consumption: Cooling Chain



Machine Plant:

- Pumps
- Chillers
- Cooling Towers
- Economizers



Data Center:

- Air Handlers
- Closely Coupled Cooling Systems
- HVAC

Back to the Desktop…

- Historically, most technologies that have appeared in high-end supercomputers have eventually migrated to the desktop
  - Hardware units for numerical computation
  - Superscalar execution
  - Parallel processing (we're observing it right now)
- In the future, it is expected that most of the technologies I presented today will eventually migrate back to desktop machines
  - High-end interconnects between cores & processors
  - Multithreading capabilities
- Commercial data centers are already looking for ways to improve their energy management