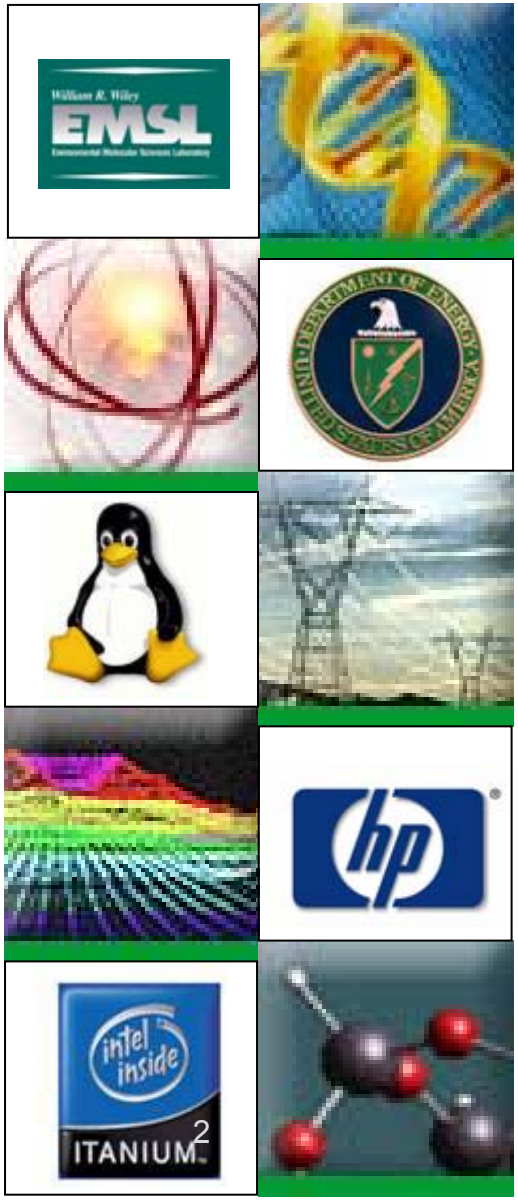

Planned Machines Panel

HPCS2 (AKA the HP cluster at PNNL)

R. Scott Studham
Molecular Science Computing Facility

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Major Applications

Largest use by far is computational chemistry (NWChem, ADF, etc.)

Note we use atomic and molecular basis sets (not grids) so many important kernels are unfamiliar to non-chemists

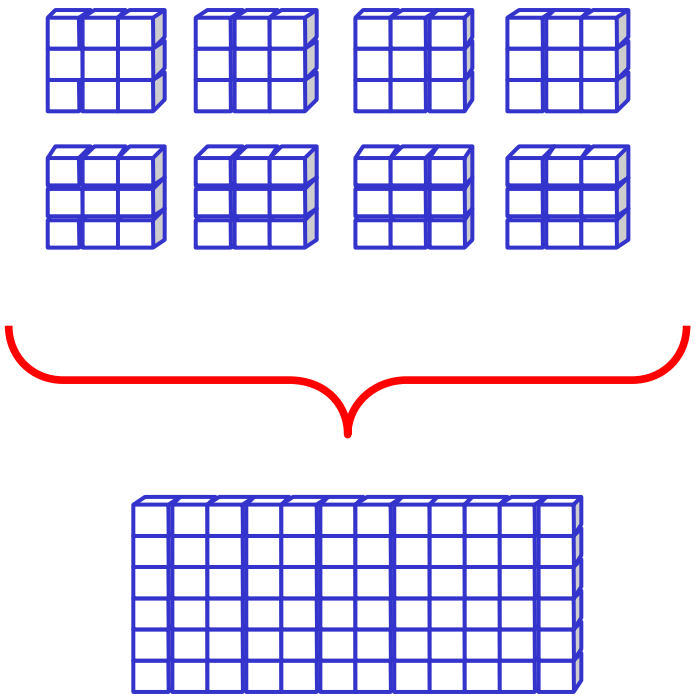
- High-accuracy electronic structure
- Low- and medium-accuracy electronic structure
- Molecular dynamics for computational biology

Other codes

- Atmospheric chemistry, regional climate modeling
- Subsurface transport
- Fluid dynamics, structural mechanics

Global Arrays

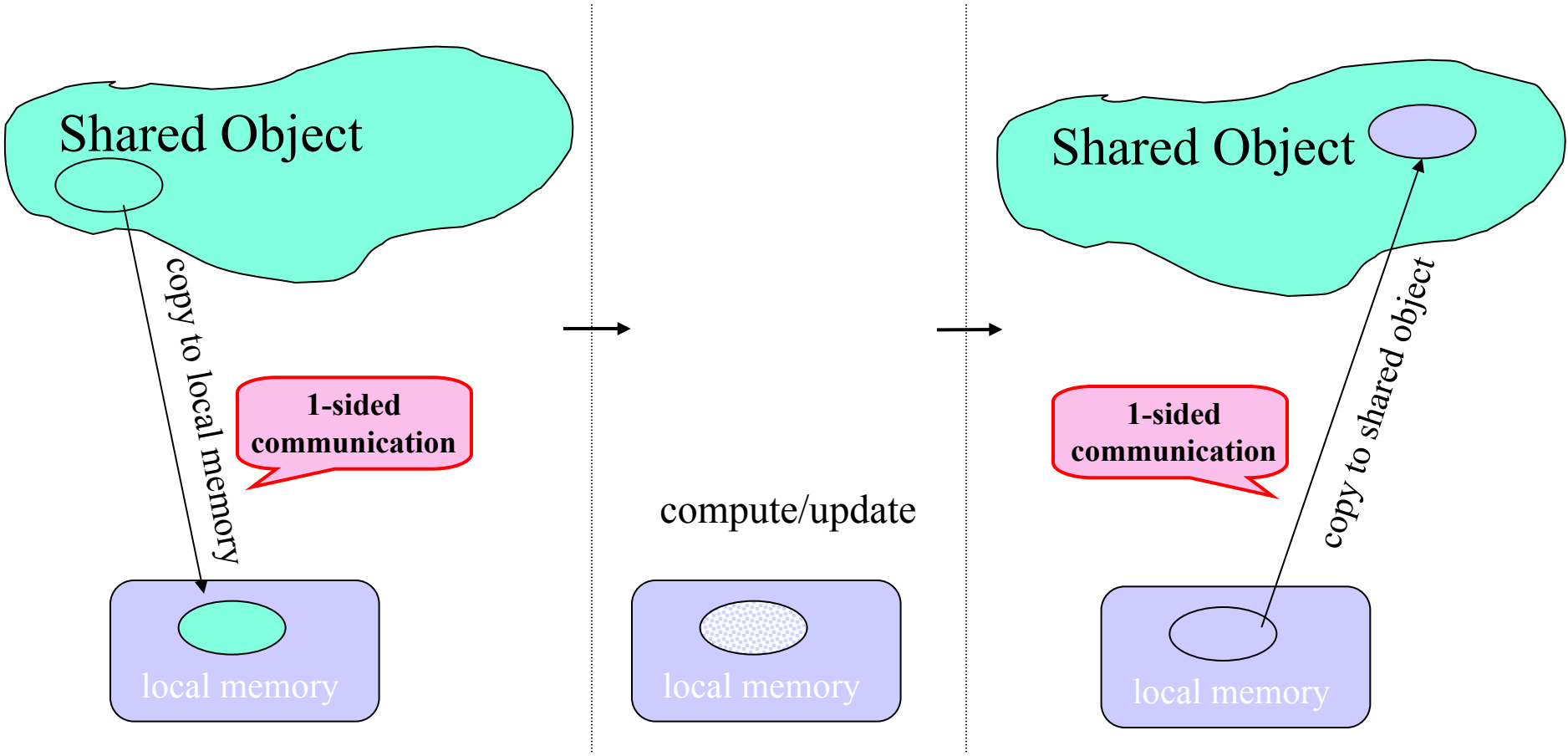
Physically distributed data



Single, shared data structure

- **Shared-memory-like model**
  - **Fast local access**
  - **NUMA aware and easy to use**
  - **MIMD and data-parallel modes**
  - **Inter-operates with MPI, …**
- **BLAS and linear algebra interface**
- **Ported to major parallel machines**
  - **IBM, Cray, SGI, clusters,...**
- **Used by most major chemistry codes, financial futures forecasting, astrophysics, CFD, computer graphics**
- **Supported by DoE MICS base program on Programming Models for Scalable Parallel Computing, and DOE 2000 ACTS in the past (J. Nieplocha)**

Shared memory model of computation in GA



- One-sided access to shared data increases ease of composition, reduces synchronization, and leads to more scalable programs

Gaussian Integral Evaluation

$$(ij\,|\,kl) = \int dr_1 dr_2 \phi_i(r_1)\phi_j(r_1) r_{12}^{-1} \phi_k(r_2)\phi_l(r_l)$$

N=O(10^3 – 10^4) – have O(N^4) integrals

Large code(s) with many critical loops

- Up to 80% of time for medium precision electronic structure calculations (SCF, DFT, MP2)
- Vectorizable recursions; short DAXPY (y(j)=a*x(j)+b*y(j)) and similar operations;
  gather and scatter; compiler generated code
- Some small level-2 and level-3 BLAS
- Tunable blocking to improve cache locality
- DAXPY-like operations must run well out of cache

SCF+MP2 analytic gradient

Semidirect algorithm

- Integrals+DGEMM+I/O
- Reduce re-computation by saving expensive AO/part transformed integrals on disk
- SCF requires high bandwidth and high capacity I/O
  - Write integrals once read many; sequential+large records
- MP2 requires lower bandwidth and less capacity
  - Out-of-core transformation/transposition
  - Strided write in blocks, sequential read
  - Blocks to use available local/shared memory and disk
  - Similar steps in coupled cluster computation

Summary of key computational kernels

CCSD(T)	DGEMM
Integrals	DAXPY-like in cache
Fock-matrix	Index eval, gather/scatter
Spectral	FFT 2-D
Mesh	Short sparse DDOT/DAXPY
MD	FFT, recip, sqrt, exp
SCF	Fast sequential IO
MP2	Fast sequential and random IO

Level-3 BLAS

DGEMM and similar operations

- Matrix multiplication
- Majority of wall time for high-precision electronic structure calculations (CCSD-T) designed to be in DGEMM
- A component of Gaussian and plane-wave DFT calculations
- Related kernels in DFT quadrature, FMM and other fast algorithms (e.g., MRA)

Achieving near theoretical peak processor speed on Itanium2 (FLAME efficiency on Itanium2)

SGEMM 99.0% of peak	CGEMM 99.0% of peak
DGEMM 98.4% of peak	ZGEMM 98.5% of peak

Let's answer Question2 then Question1.

EMSL/BER codes → Many competing algorithms, superset chosen → our balance

Q2: What characterizes your applications?

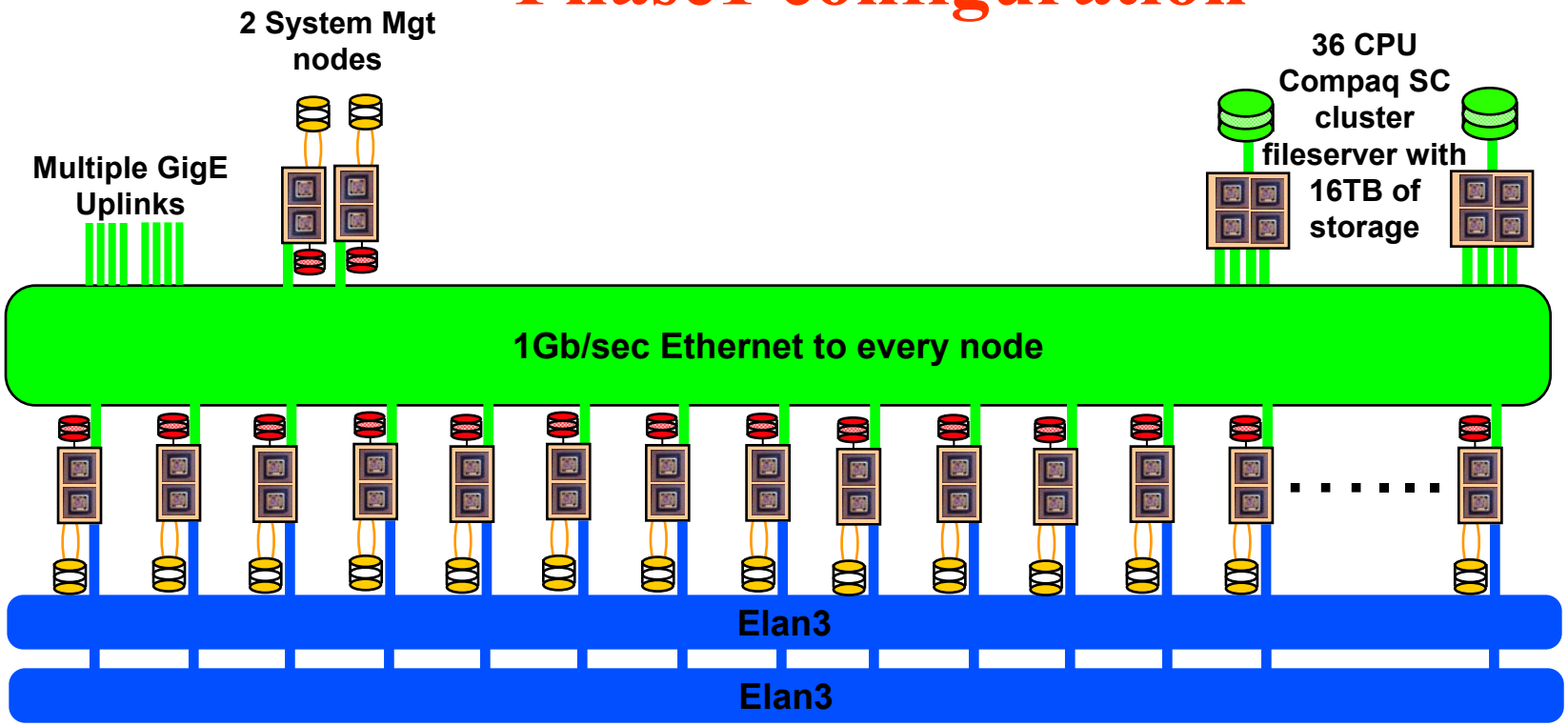
1. Global Arrays allows us to view all 7TB of RAM as a single shared object.
2. We can use local IO to cache integrals instead of recomputing
3. Applications spend large fraction of wall clock in BLAS kernels.
4. Programming models makes use of RDMA

Q1: What is unique in structure and function of your machine?

1. Require >>232 address space → 64bit everything
2. 292GB filesystem sustaining 190MB/s <u>on each node</u>
3. High efficiency in BLAS3 → Itanium2 & good math libraries
4. Quadrics Elan4 Interconnect for low latency, low overhead, RDMA.

256 Intel® Itanium® 2 processors

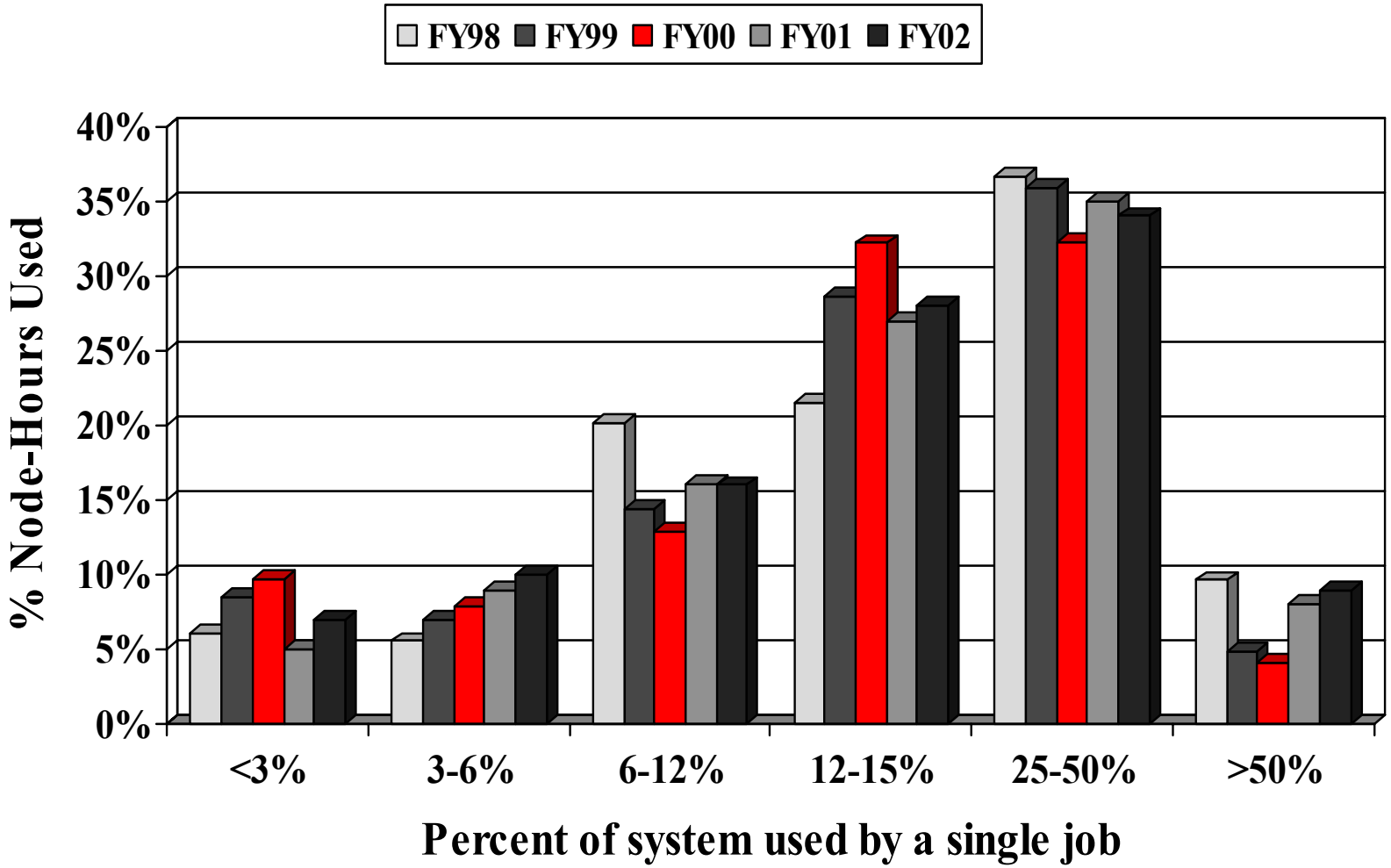
Phase1 configuration



1TF
1.5TB Memory
16TB Global FS
25GB/s Aggregate IO

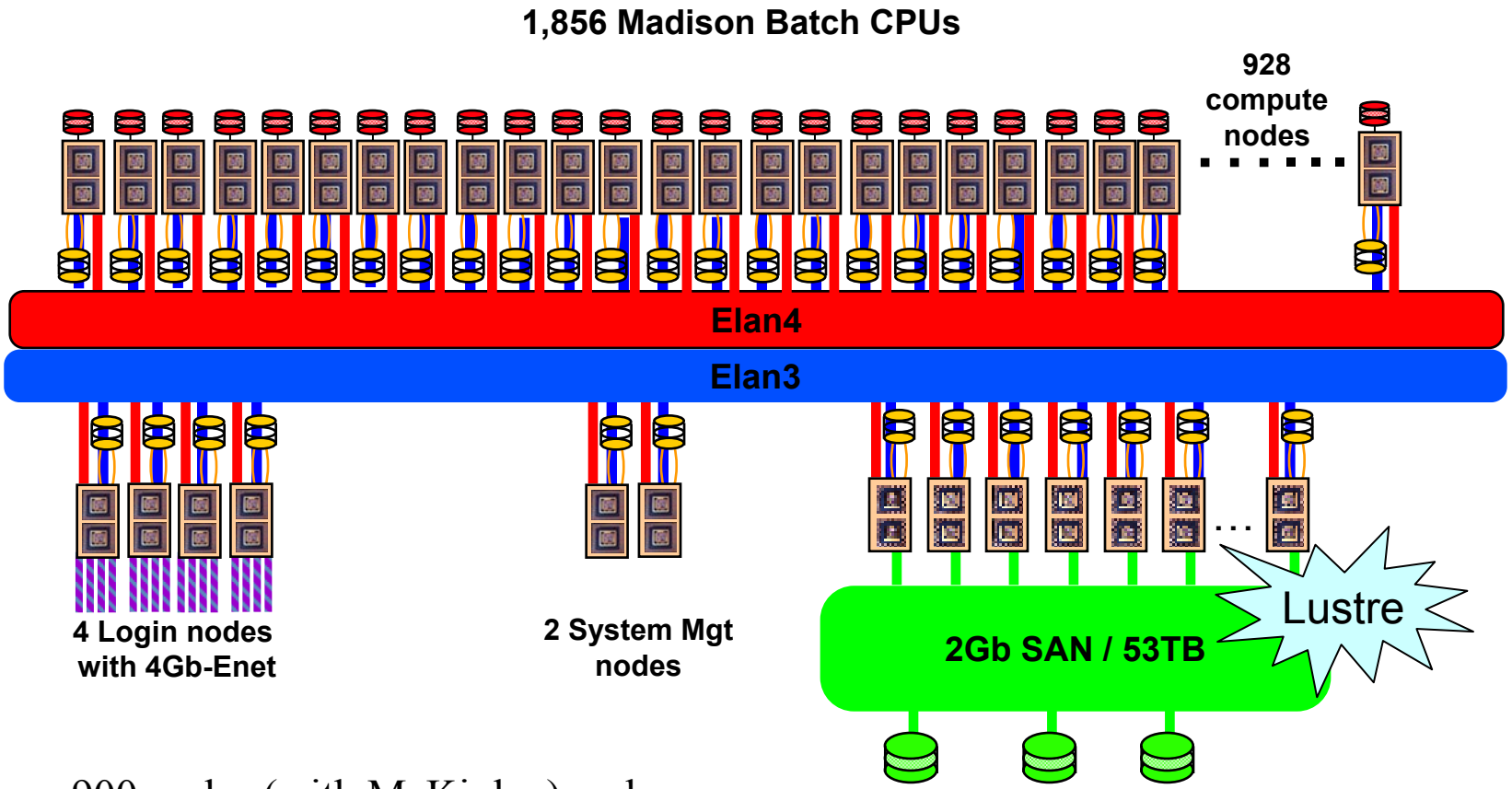
MSCF Usage

Most of the usage is in large parallel jobs



1,900+ next generation Itanium® processors

Phase2 Configuration



900 nodes (with McKinley) and Elan3 being delivered this week. Upgrade this summer.

11.4TF
6.8TB Memory

Q3: What prior experience guided you to this choice?

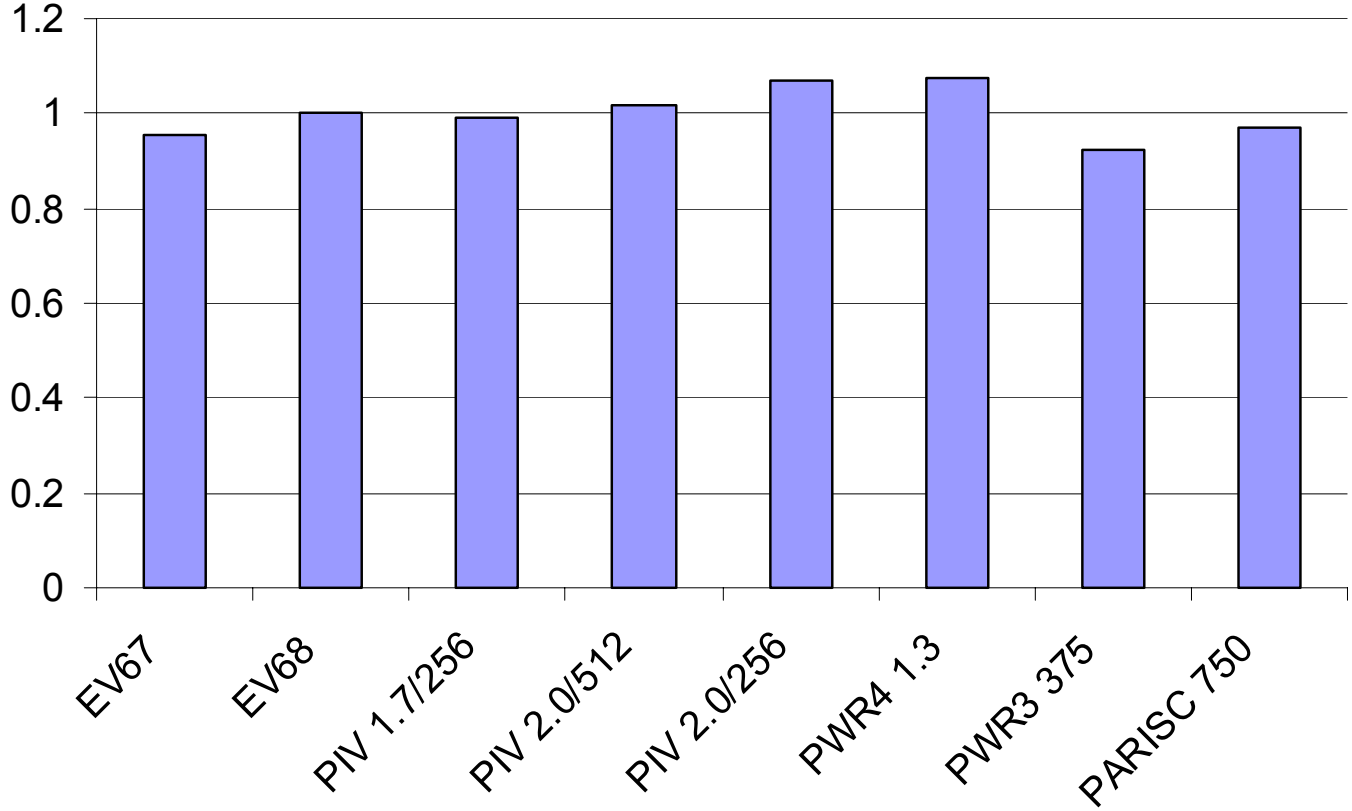
1. 512 node IBM SP2 with similar balance
   - Local IO
   - Good balance of compute to interconnect
2. Application developers were cornerstone to system choice.
3. Correlation between industry standard benchmarks and our benchmarks
4. Benchmarks on different systems with different balances.

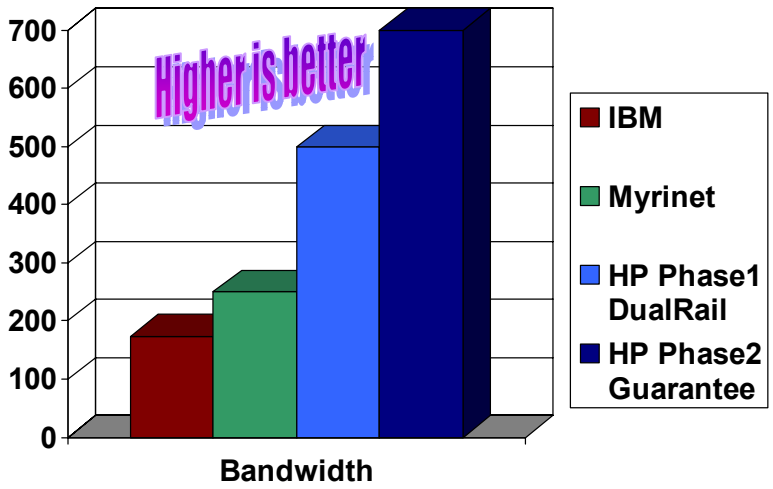
Role of Standard Benchmarks

Linpack 100/1000, SpecFP, Stream, …

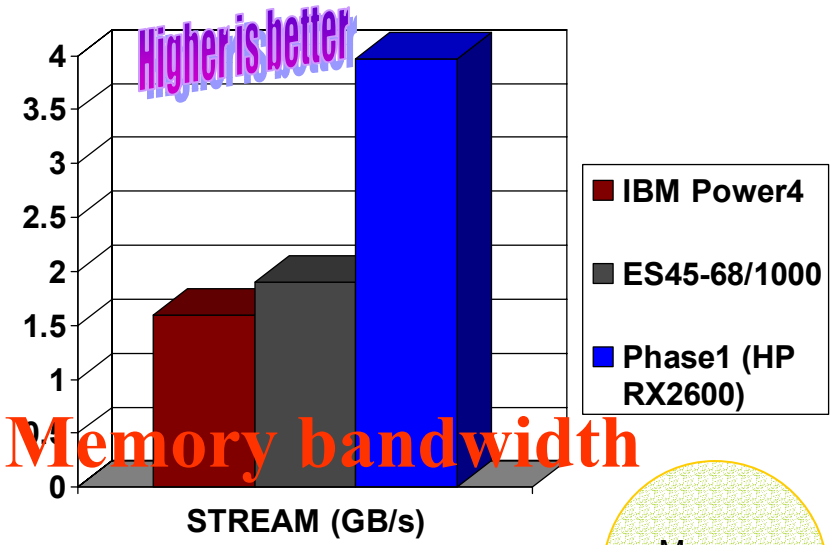
- Enable comparison between vendors with some limited interpretation
- Correlates well with selected applications
- Partially eliminates impact of immature compilers, etc.

Correlation between SpecFP and DFT SiOSi3 benchmark



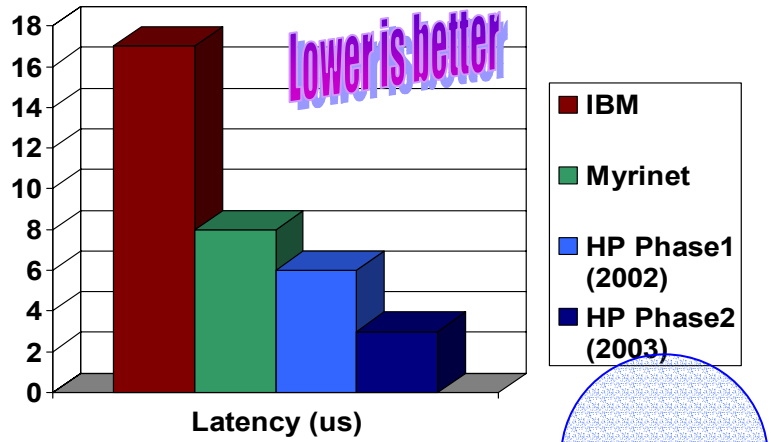


Interconnect

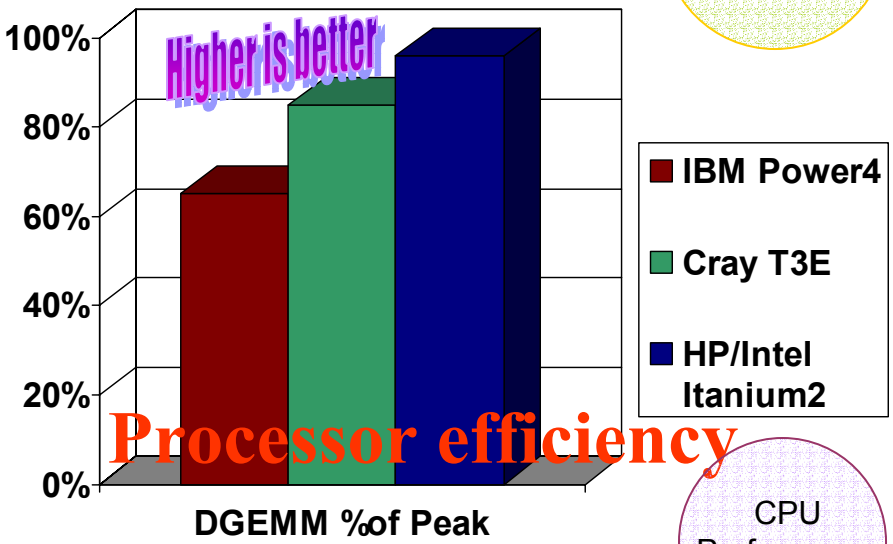


Memory bandwidth

Memory Bandwidth



Interconnect

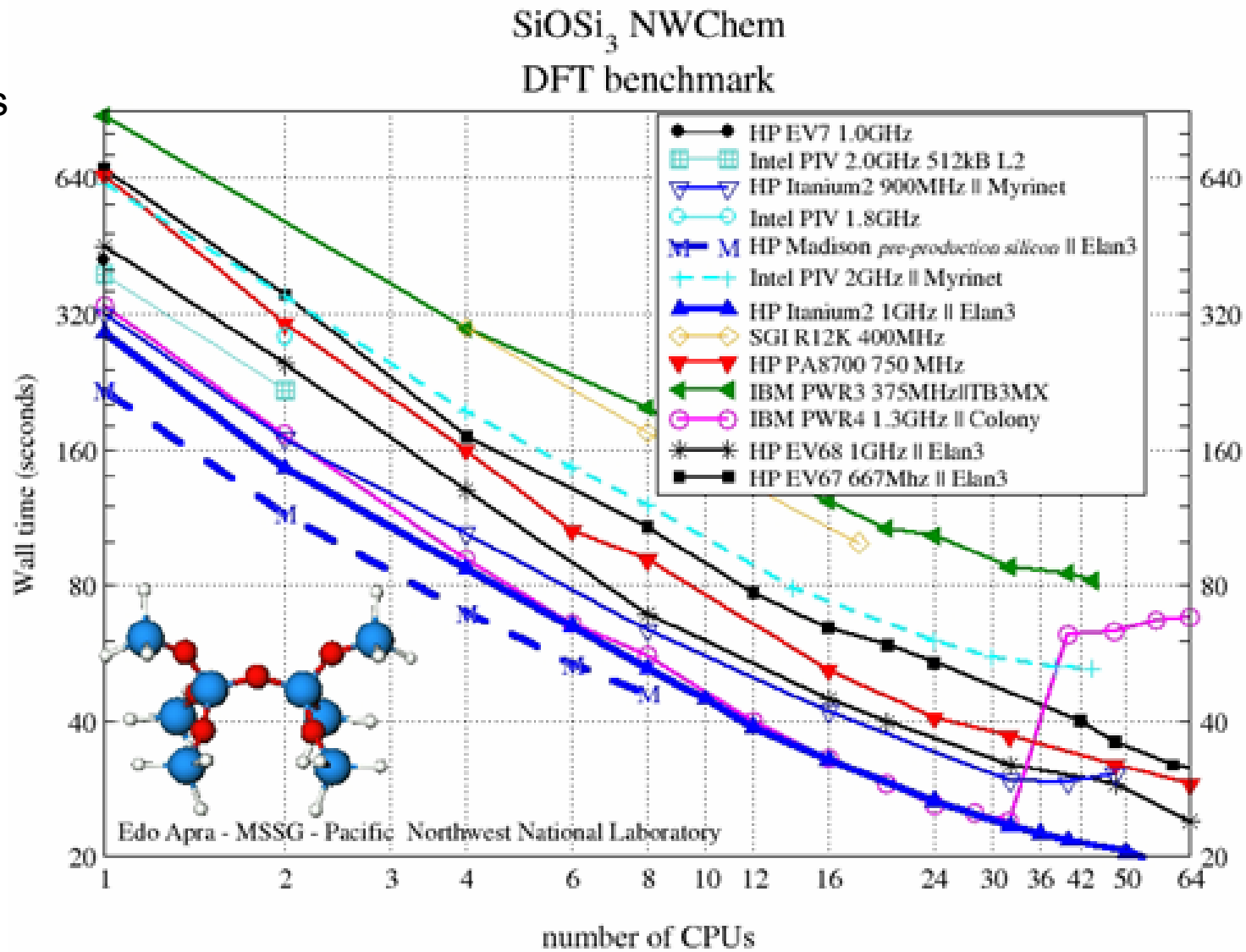


Processor efficiency

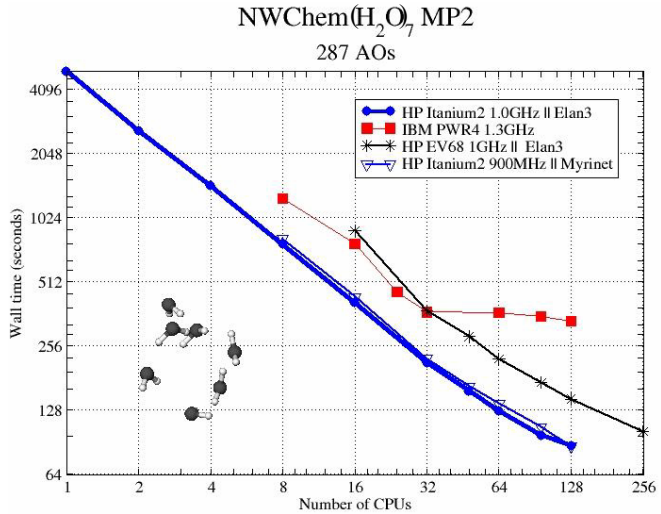
CPU Performance

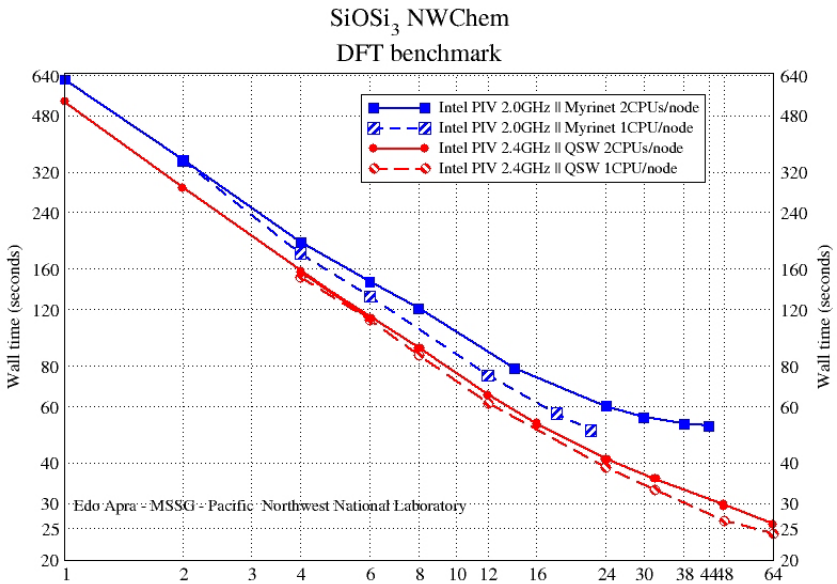
Parallel scaling of NWChem

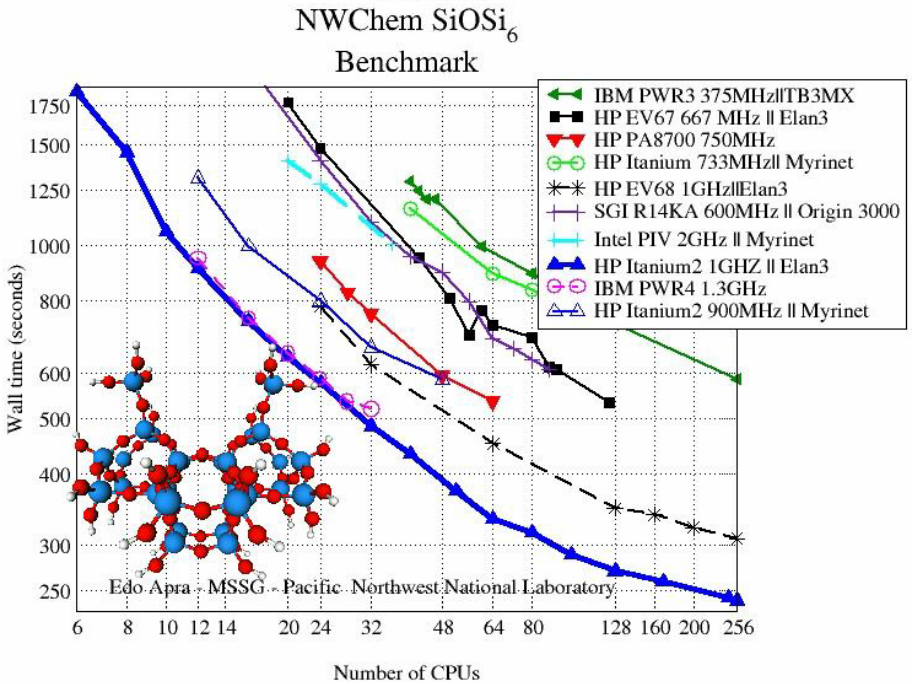
Prototype Madison's have demonstrated a greater than clock rate improvement in performance.

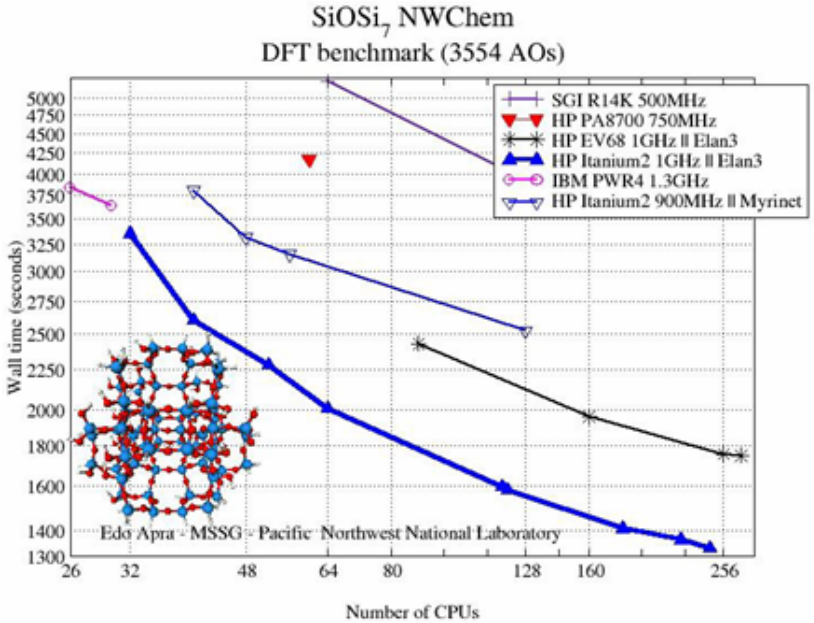


Parallel scaling of NWChem









Q4: Other than your own machine, for your needs what are the best and worst machines? And, why?

Best

EV79, Elan4 with local IO

(until somebody buys one the PSC cluster will do)

Worst

IA32, no good RDMA, without local IO

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