PERFORMANCE of VARIOUS COMPUTERS in COMPUTATIONAL CHEMISTRY

14th Daresbury Machine Evaluation Workshop
CCLRC Daresbury Laboratory

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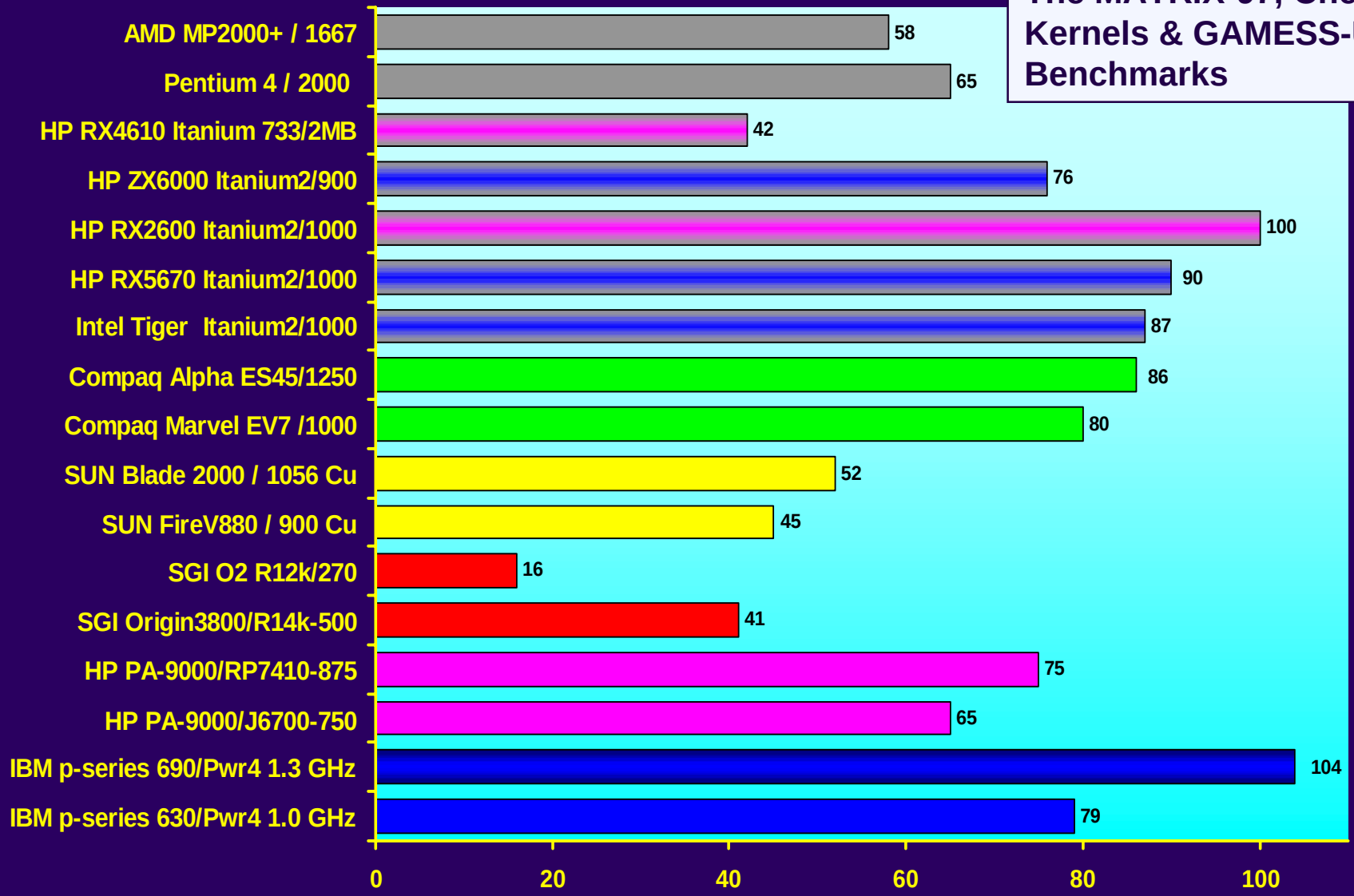
OUTLINE

- Processor Performance Overview
  - Single-processor performance, Performance Metrics
- SPEC (Standard Performance Evaluation Corporation)
  - SPEC 95 and **SPEC CPU 2000**
- Computational Chemistry Benchmark (serial) - SPECfp ?
  - Matrix and application "kernels"
  - Application packages (GAMESS-UK, DL_POLY)
  - Comparison involves 200+ computers (vector supercomputers, workstations, PCs and MPP nodes)
- Now extended to include "RATE" benchmarks
  - URLs: Powerpoint presentation and Paper:

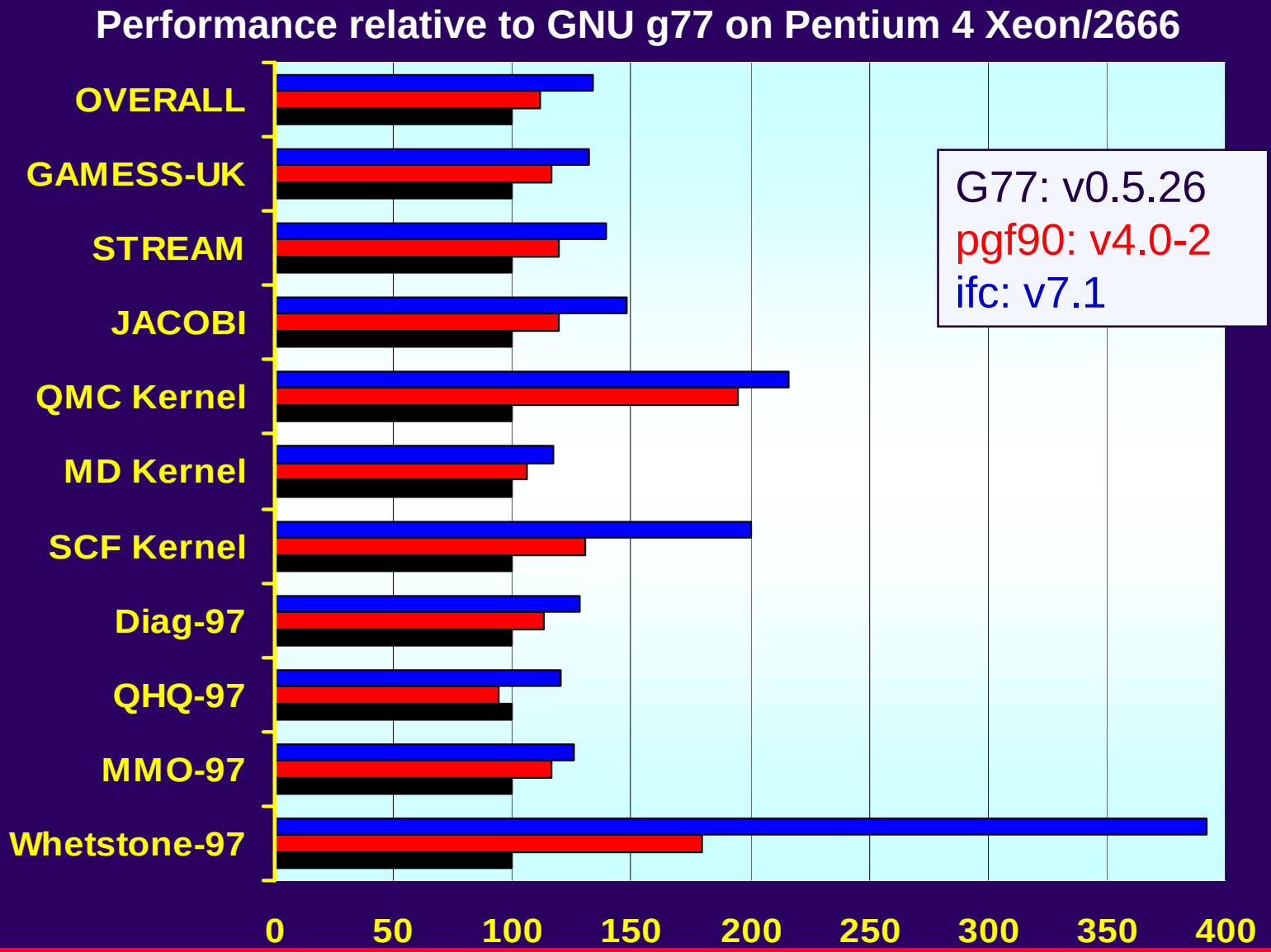
    http://www.cse.clrc.ac.uk/disco/hw-perf.shtml
- *Benchmarking of Parallel Commodity Systems*

MEW13 (2002) - Summary PI relative to the HP RX2600 Itanium2/1000

The MATRIX-97, Chemistry Kernels & GAMESS-UK Benchmarks



Fortran Compilers - Performance



MACHINES UNDER EVALUATION

Machine	Processor
AMD Athlon	MP 1.667 GHz, 2 GHz
AMD Opteron	*848 (2.2 GHz), 246 (2.0 GHz), 244 (1.8 GHz), 842 (1.6 GHz), 840 1.4 GHz*
Intel IA32	Pentium 4 2.5, 2.66 GHz, *3.06 GHz*
SUN Blade 2000 / 1056 Cu	UltraSPARC-3 / 1056 MHz
SUN Fire V880 / 900 Cu	UltraSPARC-3 / 900 MHz
HP PA-9000 / RP7410	PA8700+ / 875MHz
HP RX2600 (2-way)	Itanium 2 / 1000 MHz (3 MB L3)
HP RX5670 (4-way)	Itanium 2 / 1000 MHz (3 MB L3)
HP RX4640 (4-way)	*Itanium 2 / 1300 MHz (3 MB L3)*
HP RX2600 (2-way)	*Itanium 2 / 1500 MHz (6 MB L3)*
HP RX5670 (4-way)	*Itanium 2 / 1500 MHz (6 MB L3)*
HP ZX6000	Itanium 2 / 900 MHz (1.5 MB L3)
Intel Tiger (4-way)	Itanium 2 / 1000 MHz (3 MB L3)
Intel Tiger (4-way) +	Itanium 2 / *1200 MHz (3 MB L3)*
Intel Tiger (4-way)	Itanium 2 / *1500 MHz (6 MB L3)*

Machine	Processor
HP/Compaq ES45	AXP A21264C / 1000 MHz
HP/Compaq ES45	AXP A21264C / 1250 MHz
Compaq Marvel	EV7 1000 MHz
SGI Altix 3700	*Itanium 2 / 1300 MHz*
SGI Origin3800/R14k	R14000/R14010 600 MHz
SGI Origin300/R14k	R14000/R14010 500 MHz
SGI O2/R12k-SC	R12000/R12010 270 MHz
IBM p-Series 630	RS/6000 /POWER4 1.0GHz
IBM p-Series 690	RS/6000 /POWER4 1.3GHz
IBM p-Series 690	*RS/6000 /POWER4 1.7GHz*
Intellisation Z Pro	Itanium / 800 MHz (4 MB L3)

Vector Supercomputers

NEC SX-5, SX-4	Cray Y-MP/J90-10,
FUJITSU VPP/300,	Cray YMP C98/4256

MPP Nodes

Cray T3E/1200	AXP EV56 600 MHz
IBM SP / Power3	RS/6000 WH2 - 375 MHz

SPEC Benchmarks

NOT:
- Graphics
- Network
- I/O

- Compute intensive categories
  - integer versus floating point
  - conservative versus aggressive compilation
  - speed versus throughput
- Composite Metrics - SPEC CPU 2000

http://www.specbench.org

	SPEED	THROUGHPUT
Aggressive		
	SPECint2000	SPECint_rate2000
	SPECfp2000	SPECfp_rate2000
Conservative		
	SPECint_base2000	SPECint_rate_base2000
	SPECfp_base2000	SPECfp_rate_base2000

- SPECratio - T(measured system) / T (reference)
- Reference = 300 MHz Ultra 5/10 (100)
- SPECfp2000 - geometric mean of 14 ratios, one for each benchmark
- SPECint2000 - geometric mean of 12 ratios, one for each benchmark

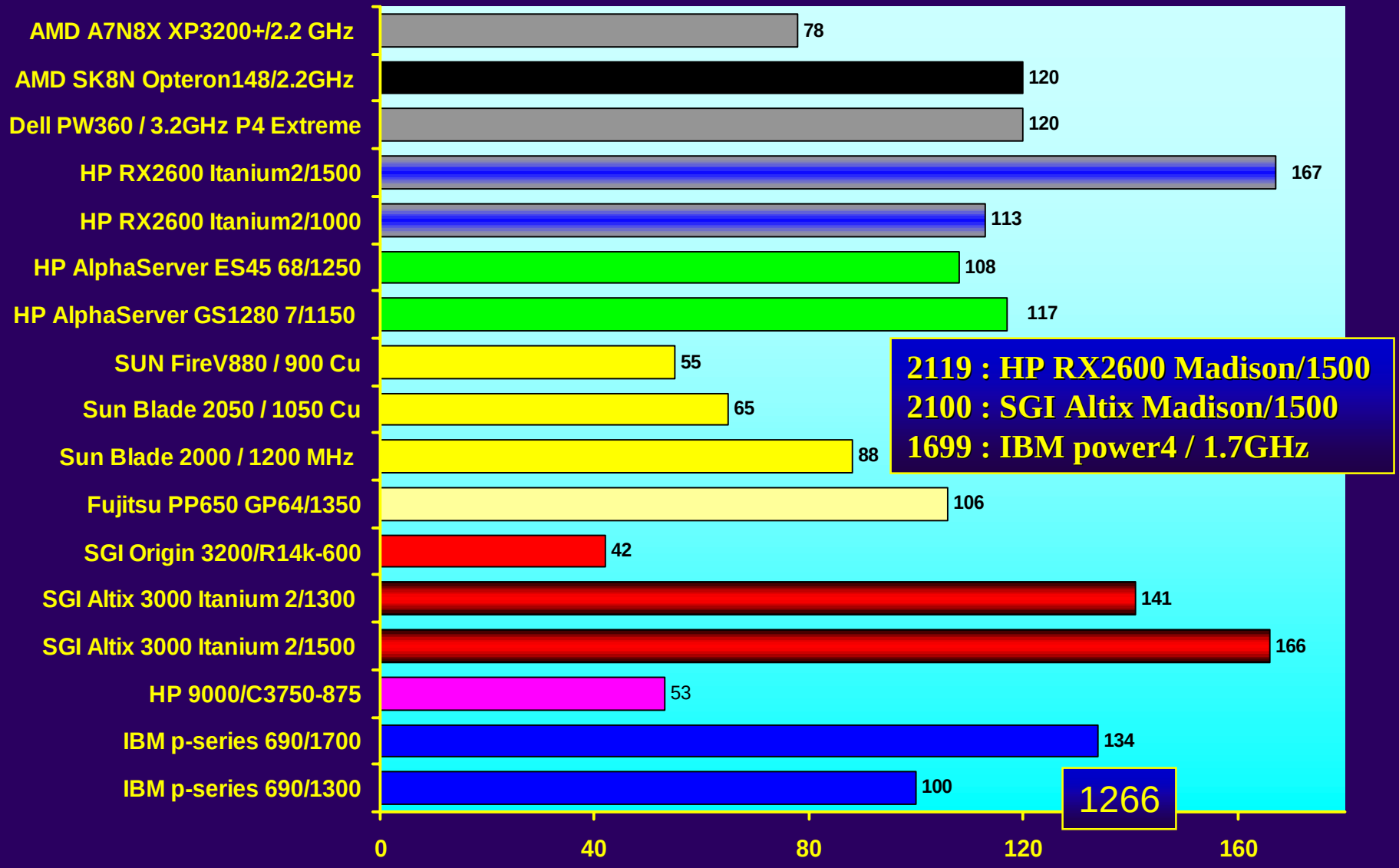
SPEC CPU 2000 - Floating point Benchmark Suite (SPECfp2000)

Benchmark	Language	Description
168.wupwise	F77	Physics: Quantum chromodynamics
171.swim	F77	Shallow water modelling
172.mgrid	F77	Multigrid solver: 3D potential field
173.applu	F77	Partial differential equations
177.mesa	C	3D graphics library
178.galgel	F90	Computational fluid dynamics
179.art	C	Image recognition / neural networks
183.equake	C	Seismic wave propagation simulation
187.facerec	F90	Image processing: Face recognition
188.ammp	C	Computational chemistry
189.lucas	F90	Number theory / primality testing
191.fma3d	F90	Finite-element crash simulation
200.sixtrack	F77	Nuclear physics accelerator design
301.apsi	F77	Metereology: Pollutant distribution

Reference: 300 MHz Ultra 5/10 = 100

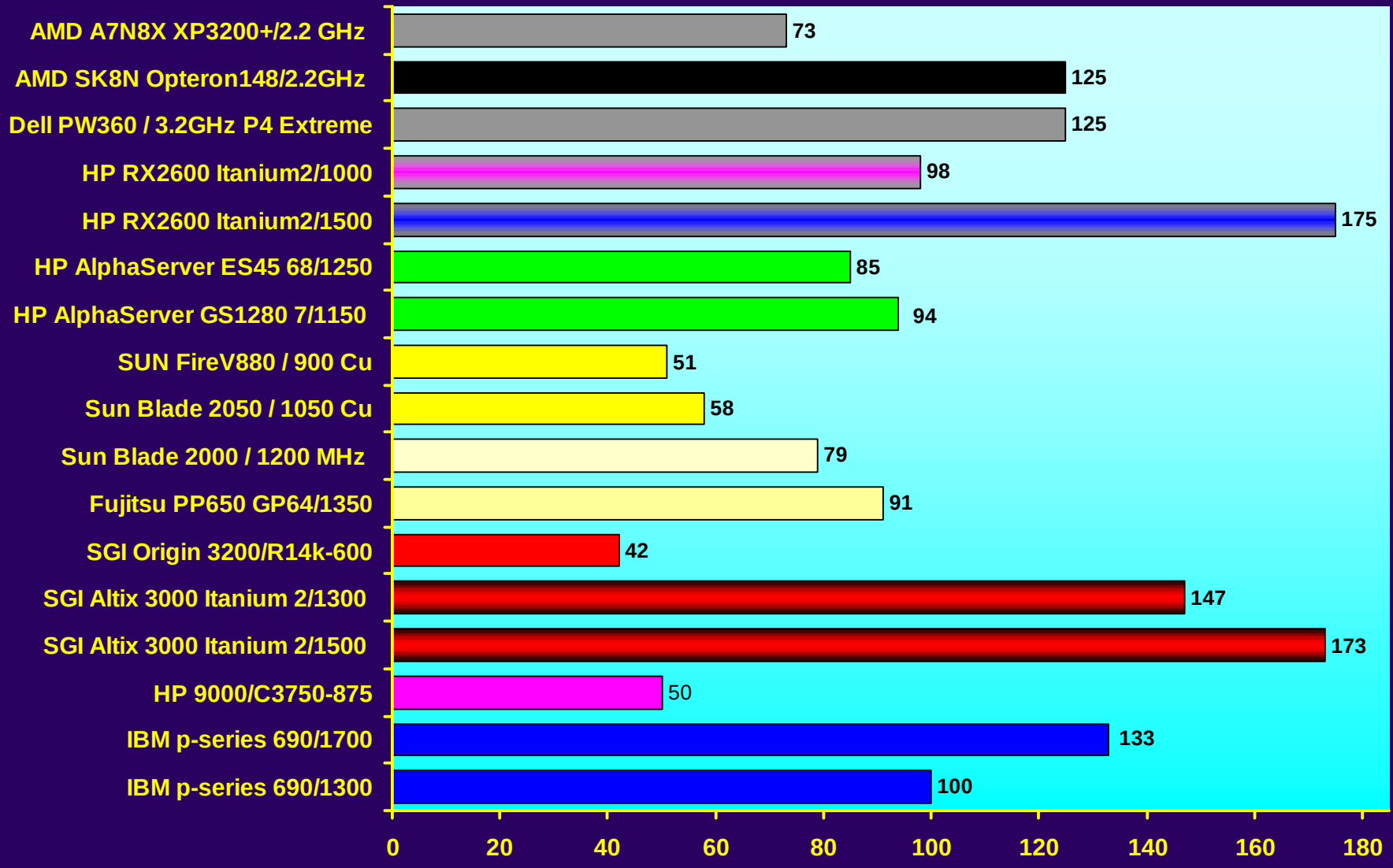
SPEC CPU 2000 - SPECfp2000

Values relative to IBM p-series 690/pwr4 1.3 GHz



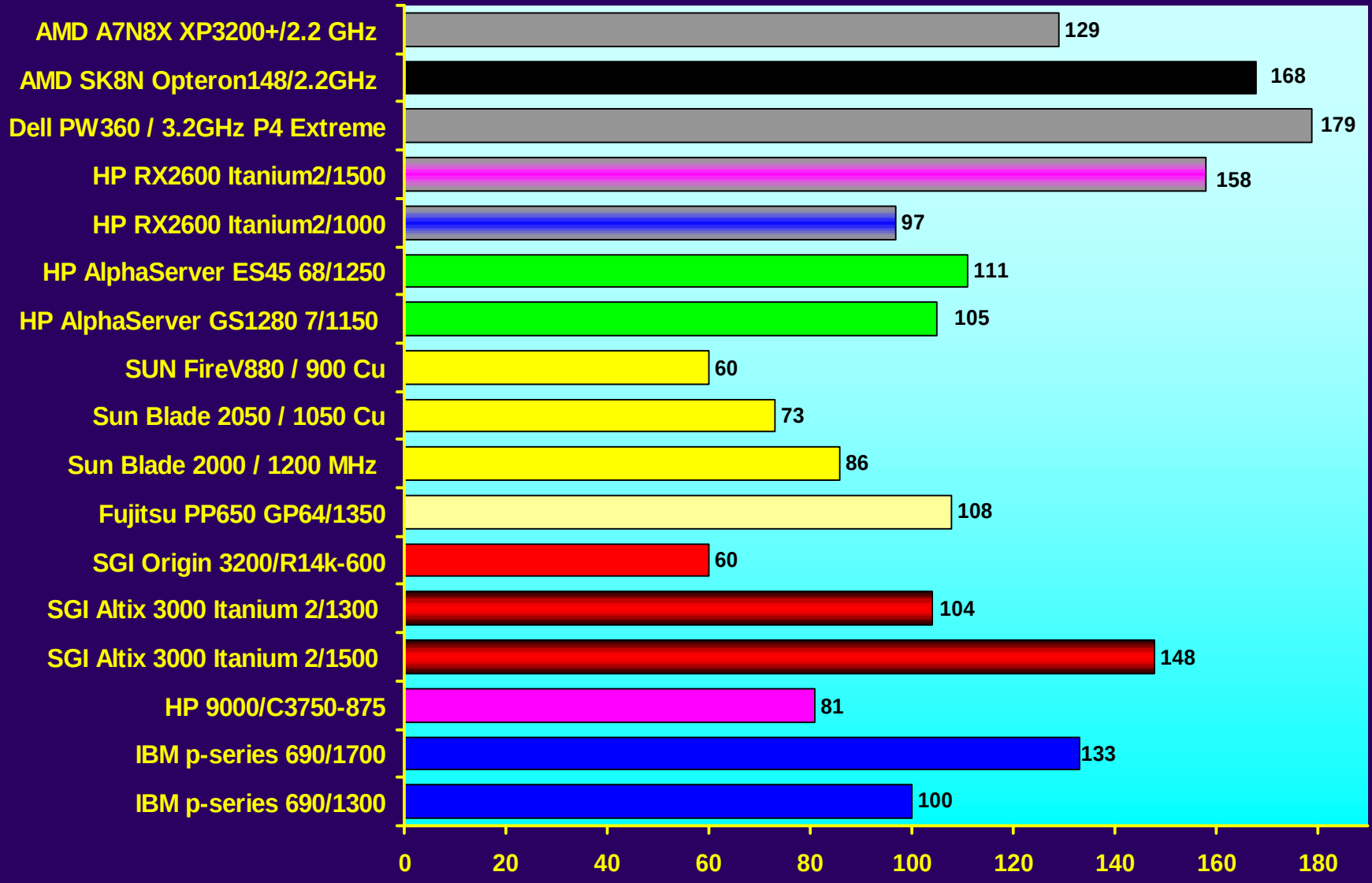
SPEC CPU 2000 - SPECfp2000_base

Values relative to IBM p-series 690/pwr4 1.3 GHz



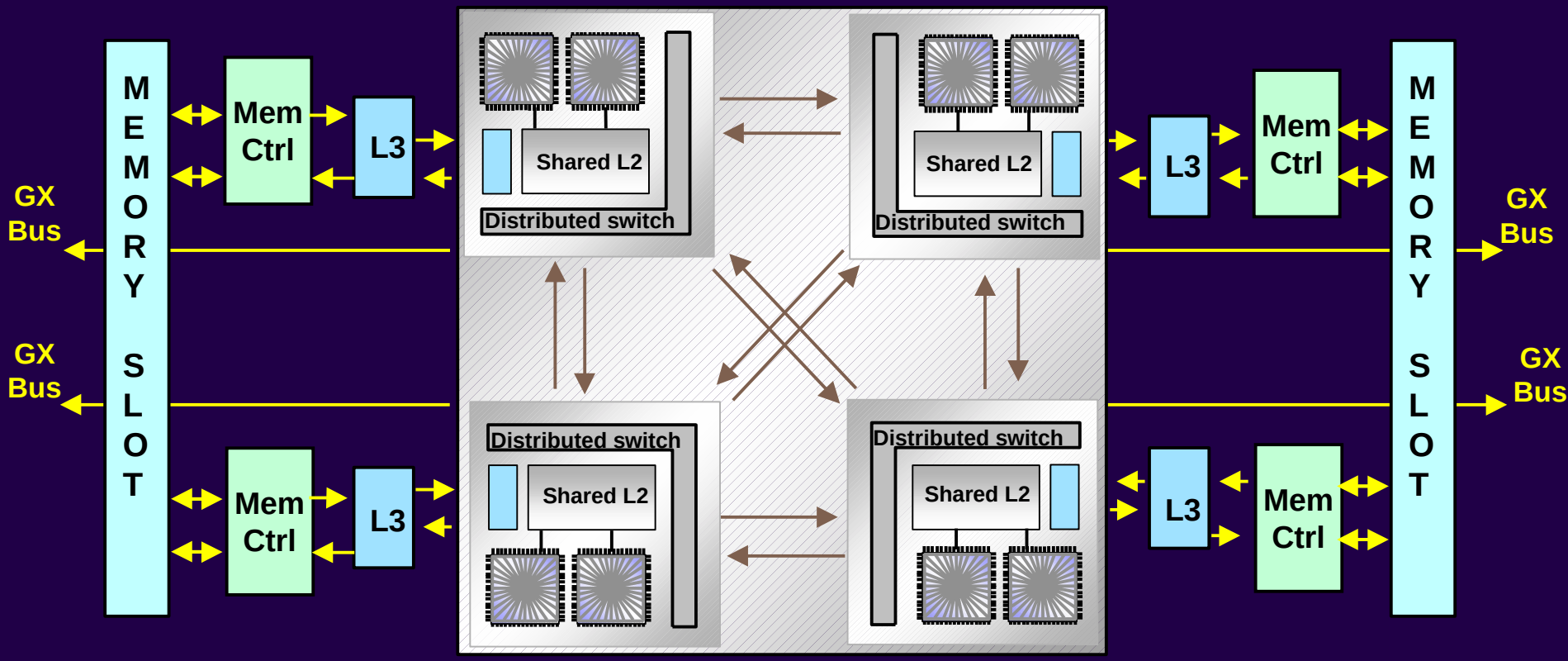
SPEC CPU 2000 - SPECint2000

Values relative to IBM p-series 690/pwr4 1.3 GHz



IBM p-series 690Turbo:Multi-chip Module (MCM)

Four POWER4 chips (8 processors) on an MCM, with two associated memory slots

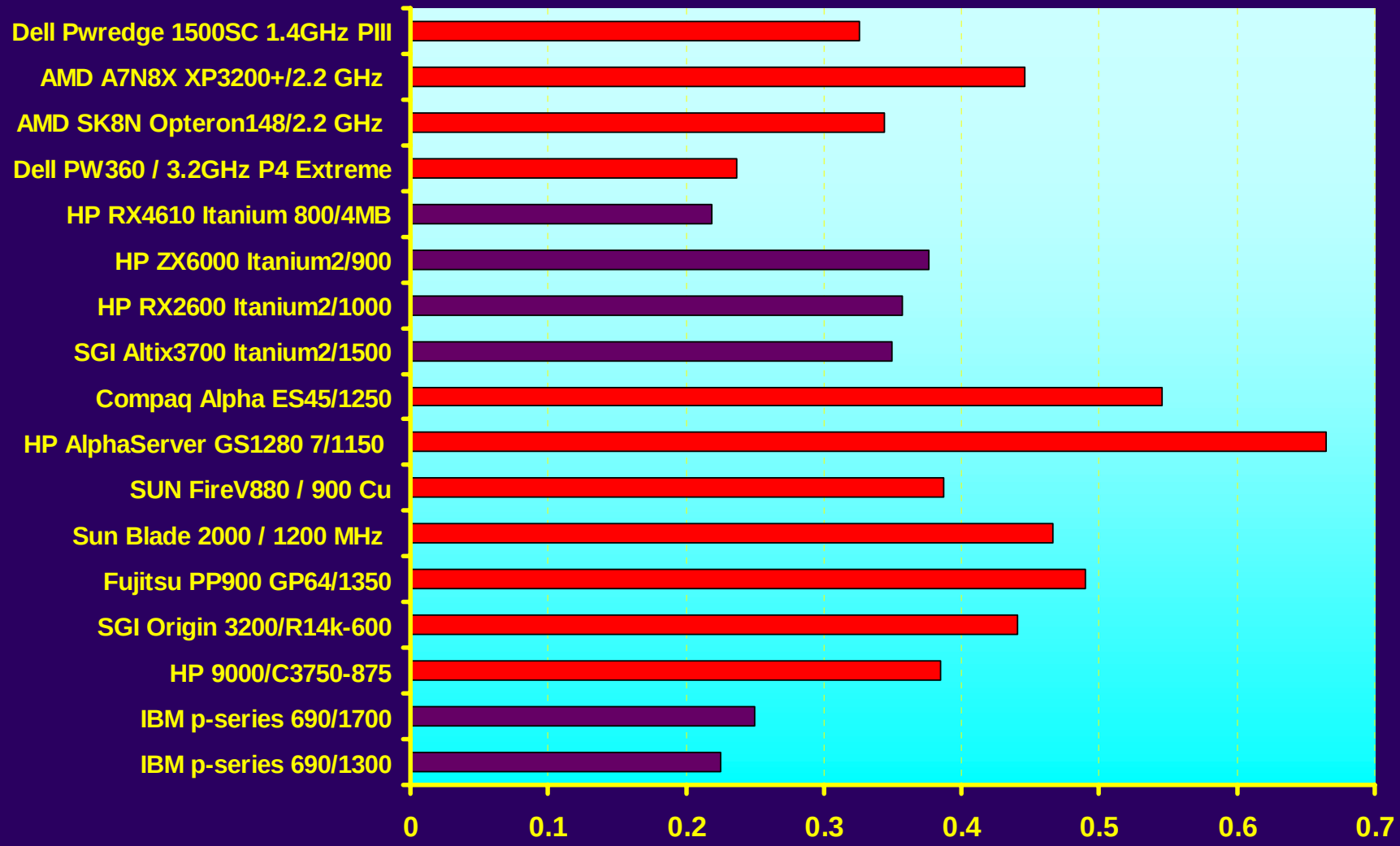


L3 cache shared across all processors

4 GX Bus links for external connections

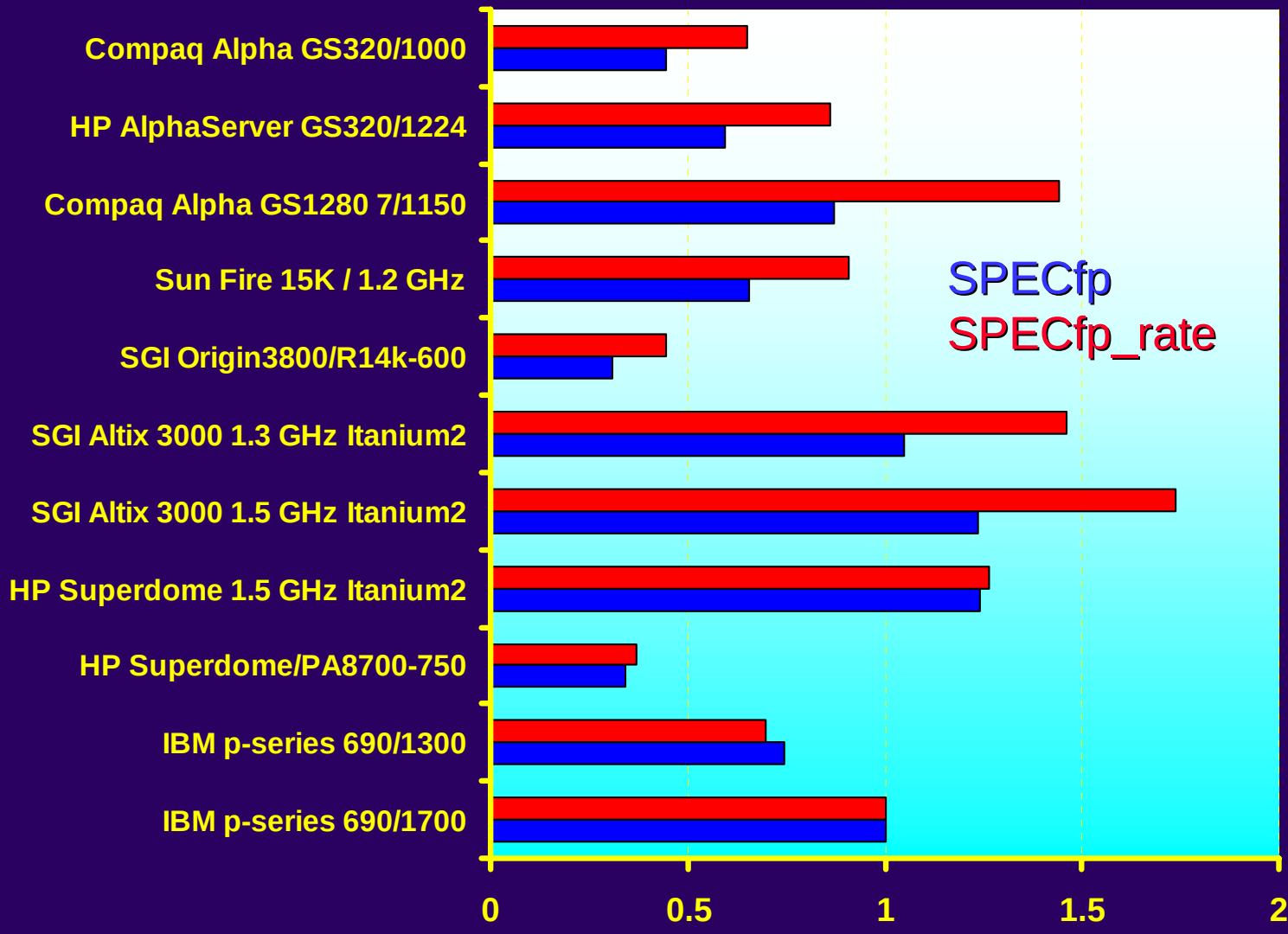
SPEC CPU 2000 - SPECfp2000

Units of SPECfp as a function of Peak Performance



SPEC CPU 2000 - SPECfp vs SPECfp_rate (32 CPUs)

Values relative to IBM 690 Turbo 1.7 GHz



Computational Chemistry Benchmark Suite

- Benchmark suite developed to incorporate:
  - Matrix “kernels” (MATRIX-89 and MATRIX-97)
  - Application “kernels”
  - Application packages (e.g. GAMESS-UK, DL_POLY)
- Implemented on Supercomputers, servers (superminis), workstations, PCs and parallel machines
  - Matrix Operations / Matrix multiplication and matrix diagonalisation
  - Computational Chemistry Kernels - four typical application kernels (direct-SCF, MD, QMC and Jacobi eigen solver)
  - STREAM (memory bandwidth)
  - Quantum Chemistry Calculations - twelve typical applications, including SCF, direct-SCF, CASSCF, MCSCF, direct-CI and MRD-CI, MP2, 2nd derivatives (GAMESS-UK-89 and GAMESS-UK-99)
  - Molecular Dynamics Calculations - six typical simulations

COMPUTATIONAL CHEMISTRY BENCHMARKS I. Matrix Operations

MATRIX OPERATIONS (MATRIX-89 and MATRIX-97)

- SPARSE Matrix Multiply BenchMark
  - MMO operation is central to the efficient operation of modern QC codes. In this benchmark a series of MMOs (R = A X B) are performed involving matrices of increasing order:
    - MATRIX-89: 10, 20, 30, … , 100 (B is sparse)
    - MATRIX-97: 50, 100, 150, … , 500 (B is sparse)

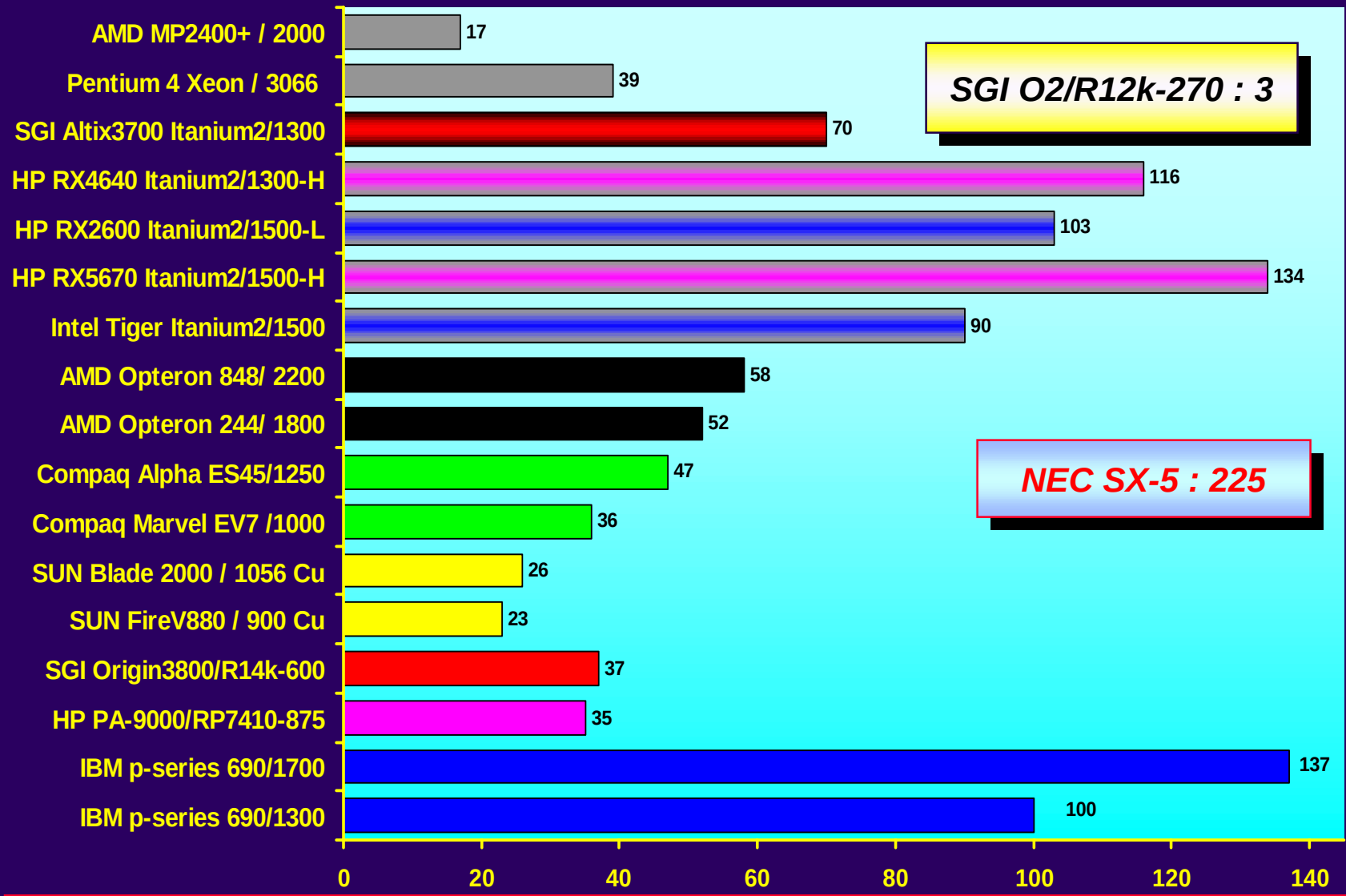
Memory bandwidth

- Diagonalisation Benchmark
  - Based on diagonalising a series of real symmetric matrices. Measures the performance of 8 routines from mathematical libraries and QC codes:
    - MATRIX-89: 10, 20, 30, … , 100
    - MATRIX-97: 50, 100, 150, 200, 250, 300
- $Q^{\dagger}HQ$ Benchmark
  - Designed to extend MMO benchmark by allowing for the use of library routines e.g. BLAS. Uses both a scalar and vector algorithm:
    - MATRIX-89: 10, 20, 30, … , 150
    - MATRIX-97: 20, 40, 60, … , 300

-lblas

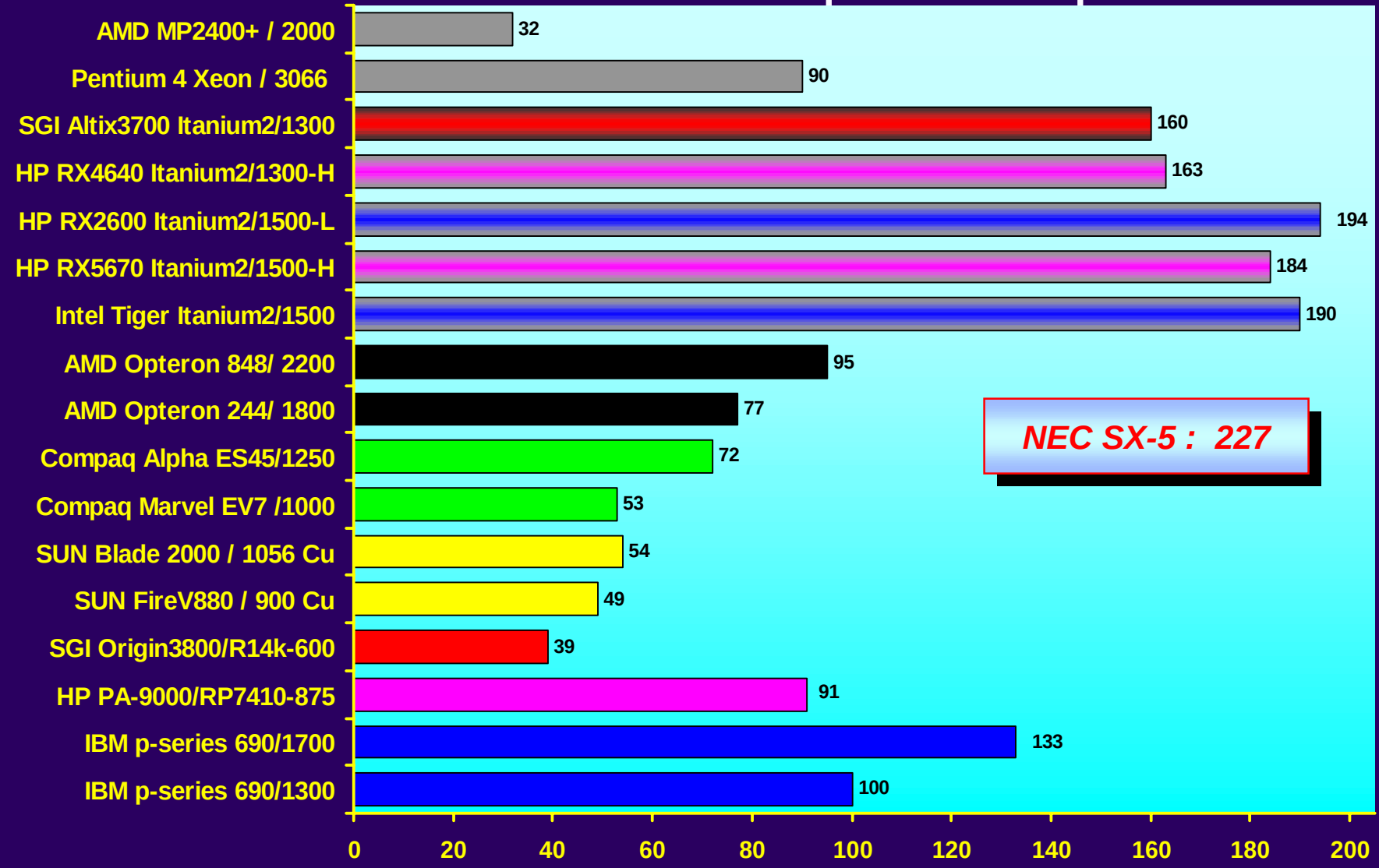
Matrix-97: SPARSE MMO Benchmark.

Performance relative to the IBM p-series 690/pwr4 1.3 GHz



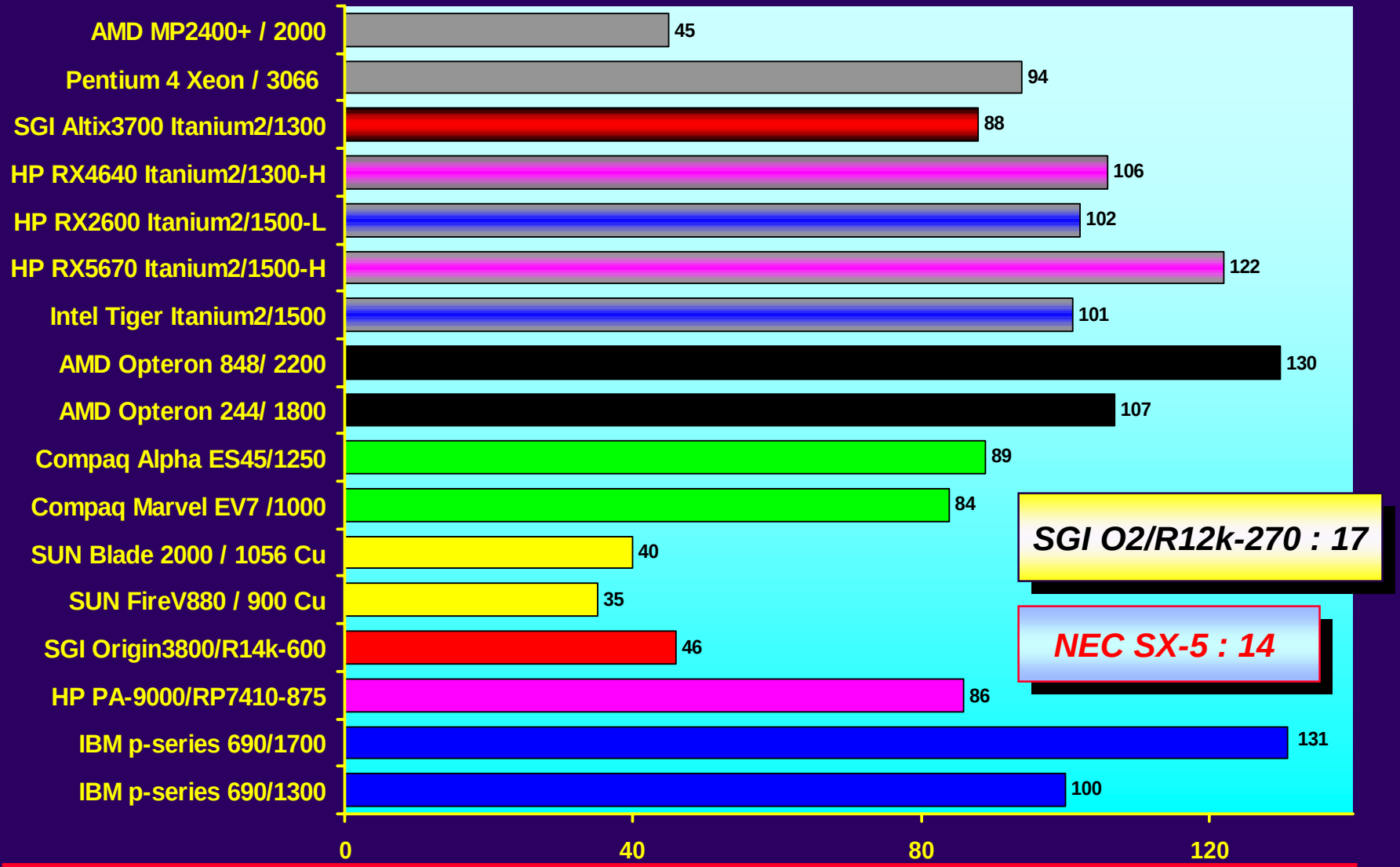
Matrix-97: Q†HQ MMO Benchmark.

Performance relative to the IBM p-series 690/pwr4 1.3 GHz



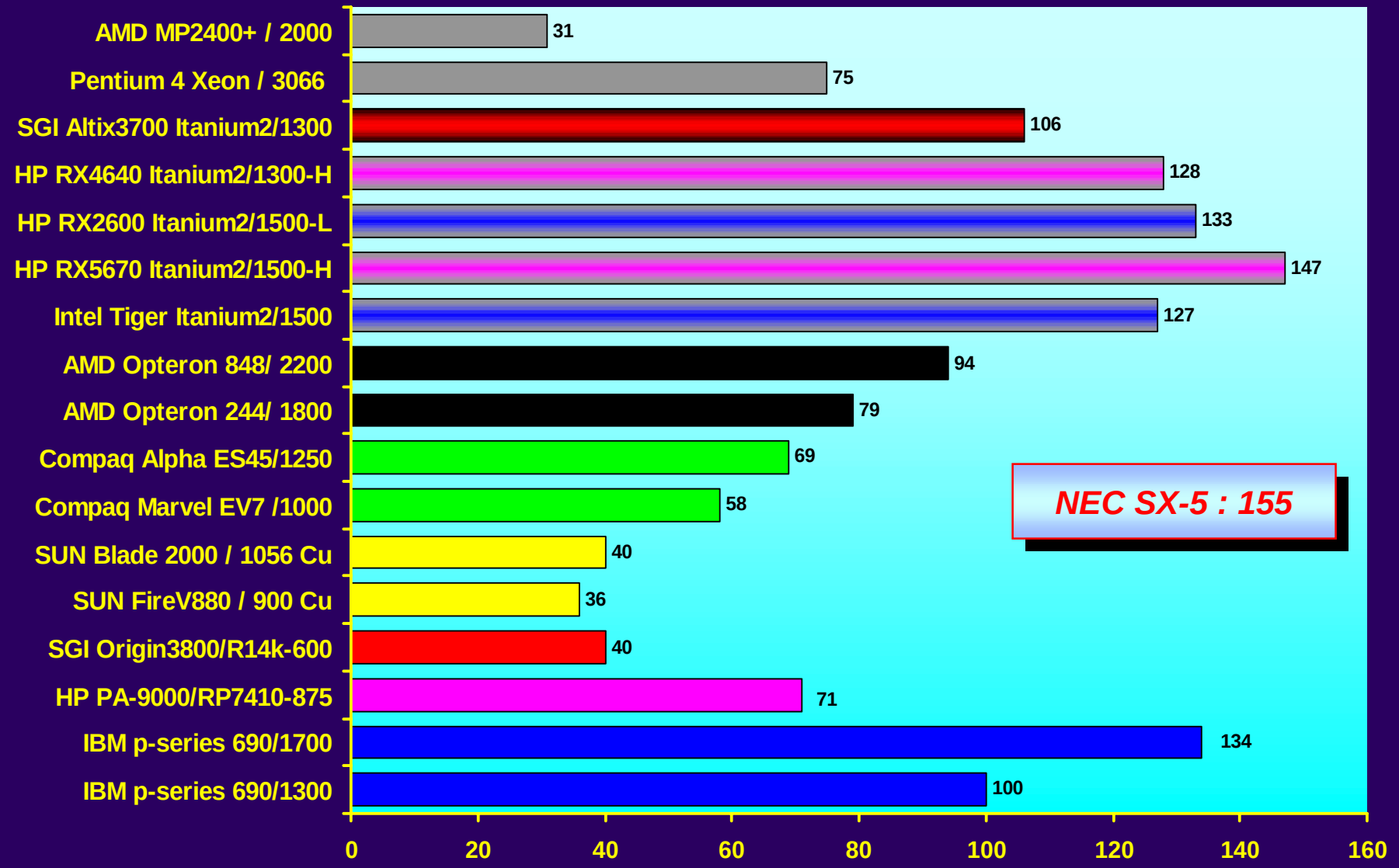
Matrix-97: Diagonalisation Benchmark

Performance relative to the IBM p-series 690/pwr4 1.3 GHz



The Matrix-97 Benchmarks.

Performance relative to the IBM p-series 690/pwr4 1.3 GHz



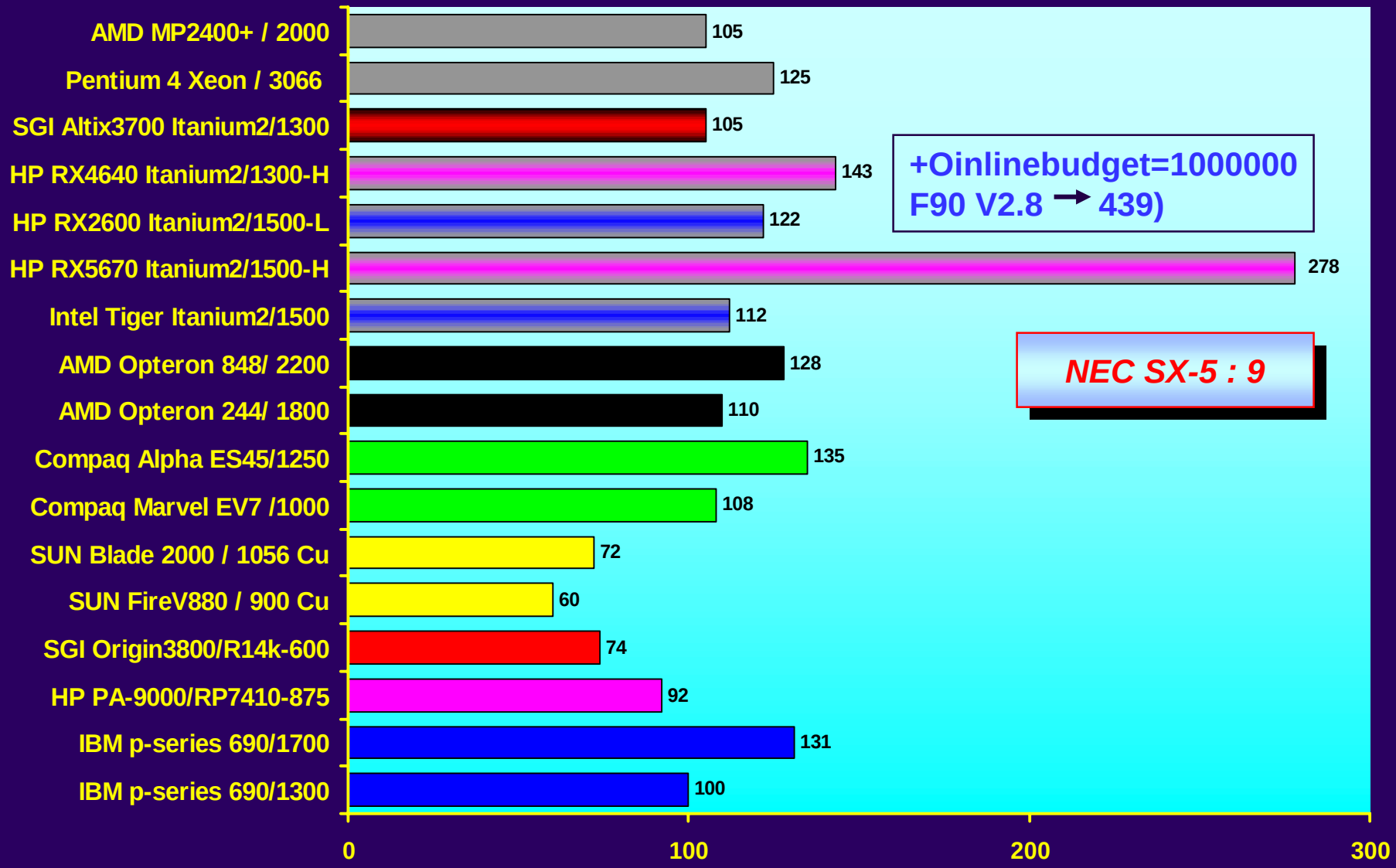
COMPUTATIONAL CHEMISTRY KERNELS

Programs that are realistic models of actual chemical applications or algorithms

- Self consistent Field (SCF)
  - SCF code using distributed primitive 1s gaussian functions as a basis (thus emulating the use of s, p, functions); performs direct-SCF calculation on Be_4 (60 functions).
- Molecular Dynamics (MD)
  - This code bounces a few thousand argon atoms around in a box with periodic boundary conditions. LJ pair-wise interactions are used with integration of the Newtonian equations of motion.
- Quantum Monte Carlo (QMC)
  - This code evaluates the energy of the simplest explicitly correlated electronic wavefunction for the He atom using a variational monte-carlo method without importance sampling.
- Jacobi iterative linear equation solver (JACOBI)
  - JACOBI uses a naive jacobi iterative algorithm to solve a linear equation. All the time is spent in a large matrix-vector multiplication.

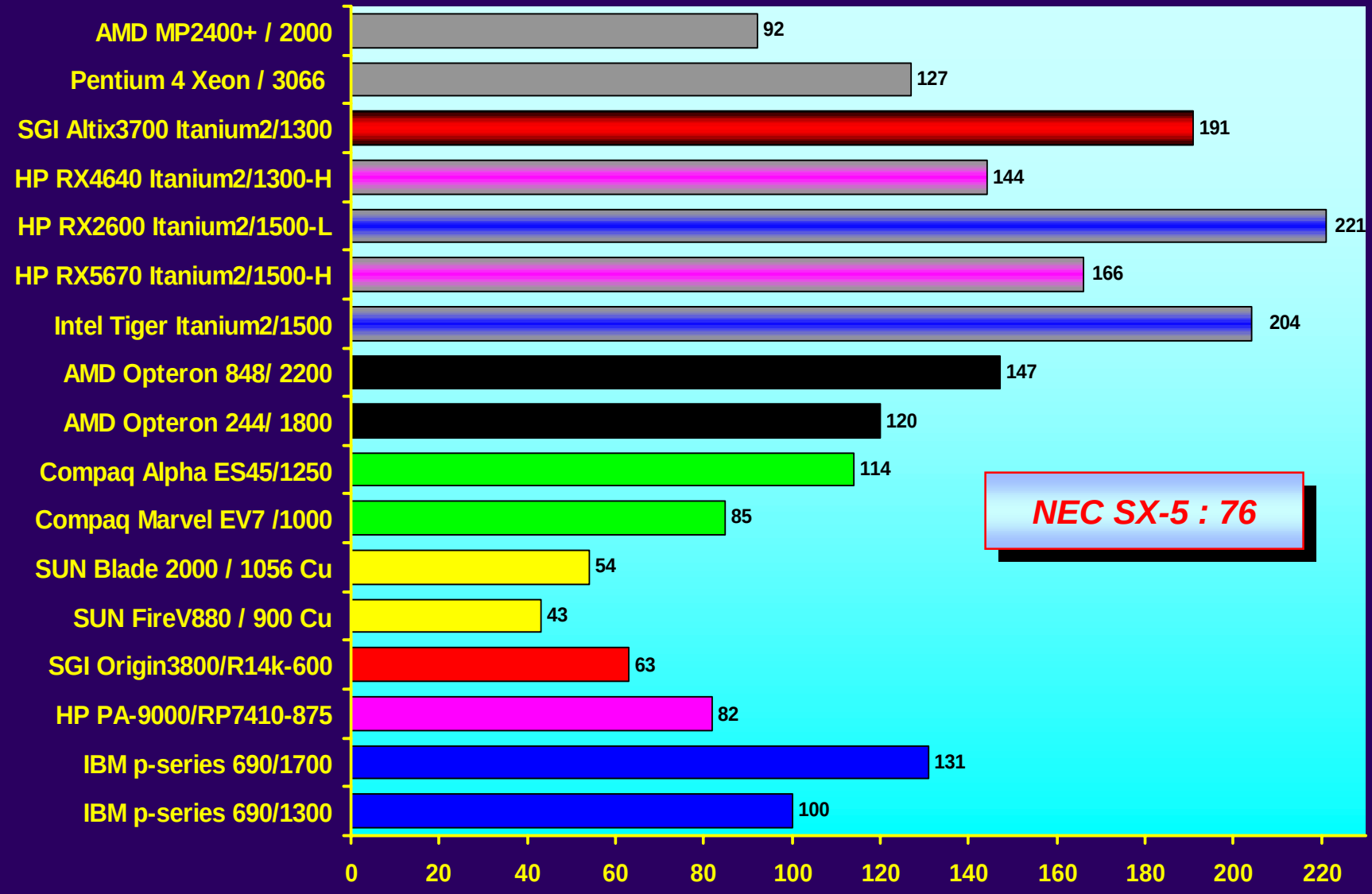
Computational Chemistry Kernels - Direct-SCF.

Performance relative to the IBM p-series 690/pwr4 1.3 GHz



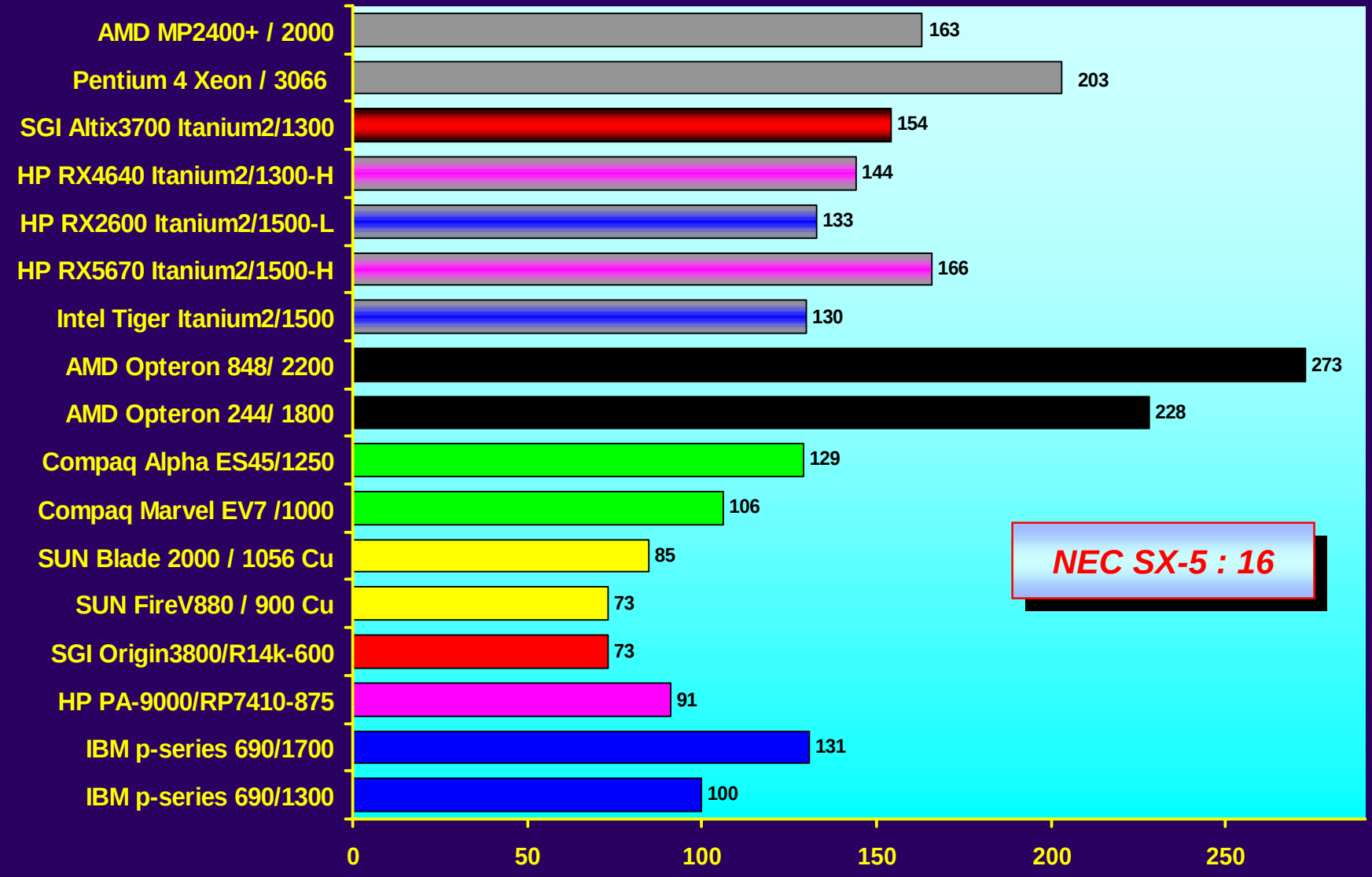
Chemistry Kernels - Molecular Dynamics.

Performance relative to the IBM p-series 690/pwr4 1.3 GHz



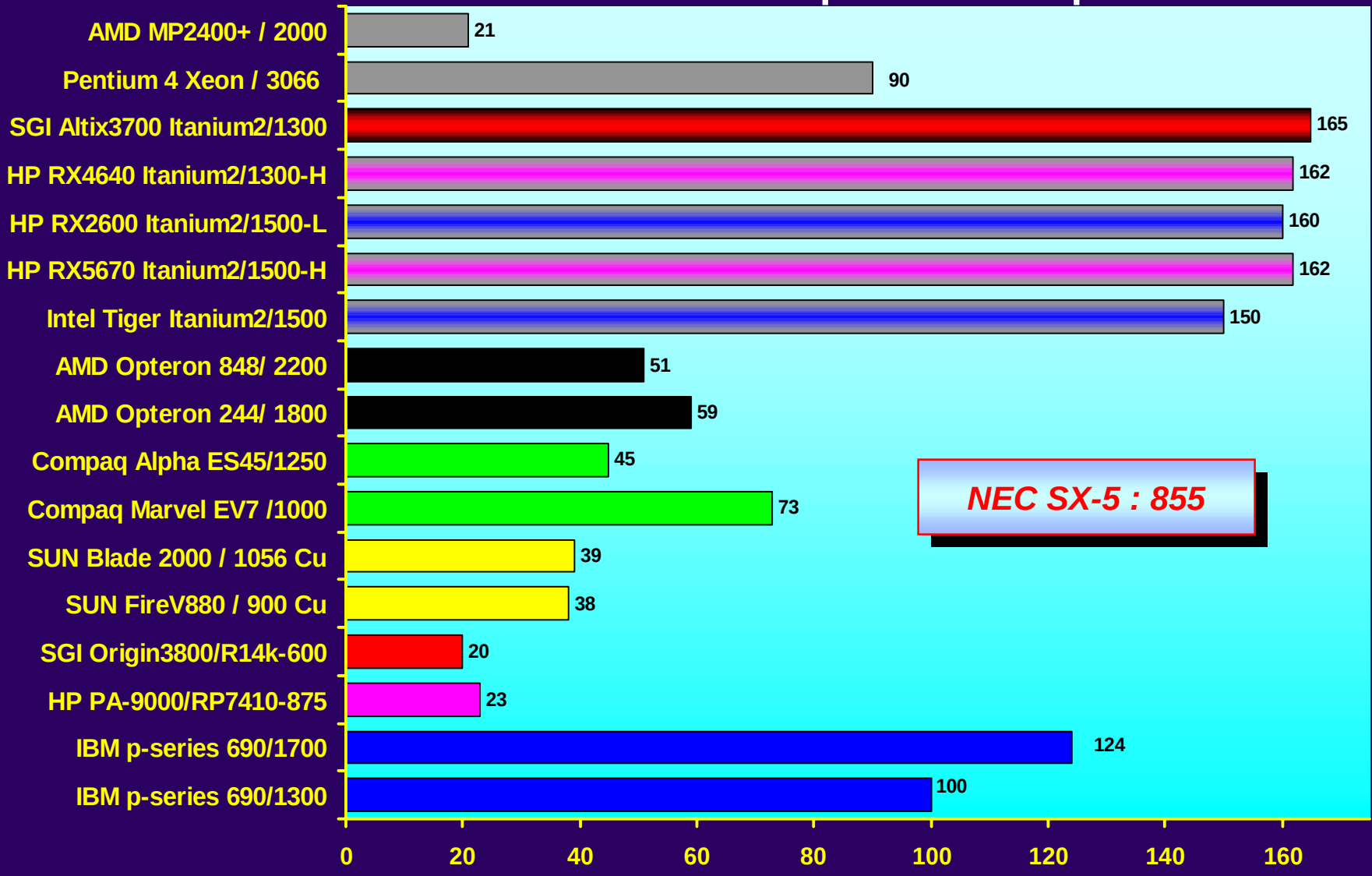
Chemistry Kernels - Quantum Monte Carlo.

Performance relative to the IBM p-series 690/pwr4 1.3 GHz

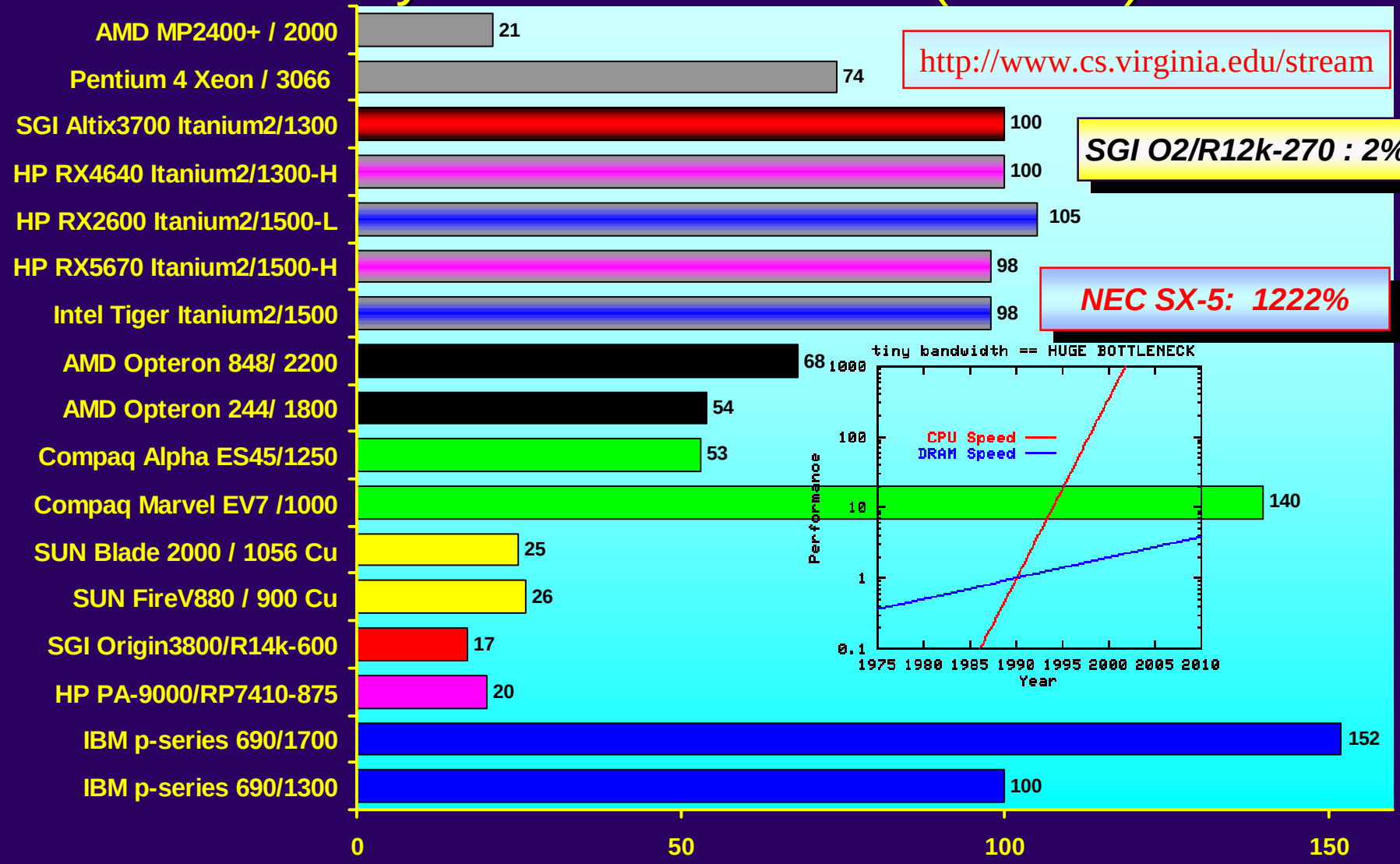


Chemistry Kernels - Jacobi Solver.

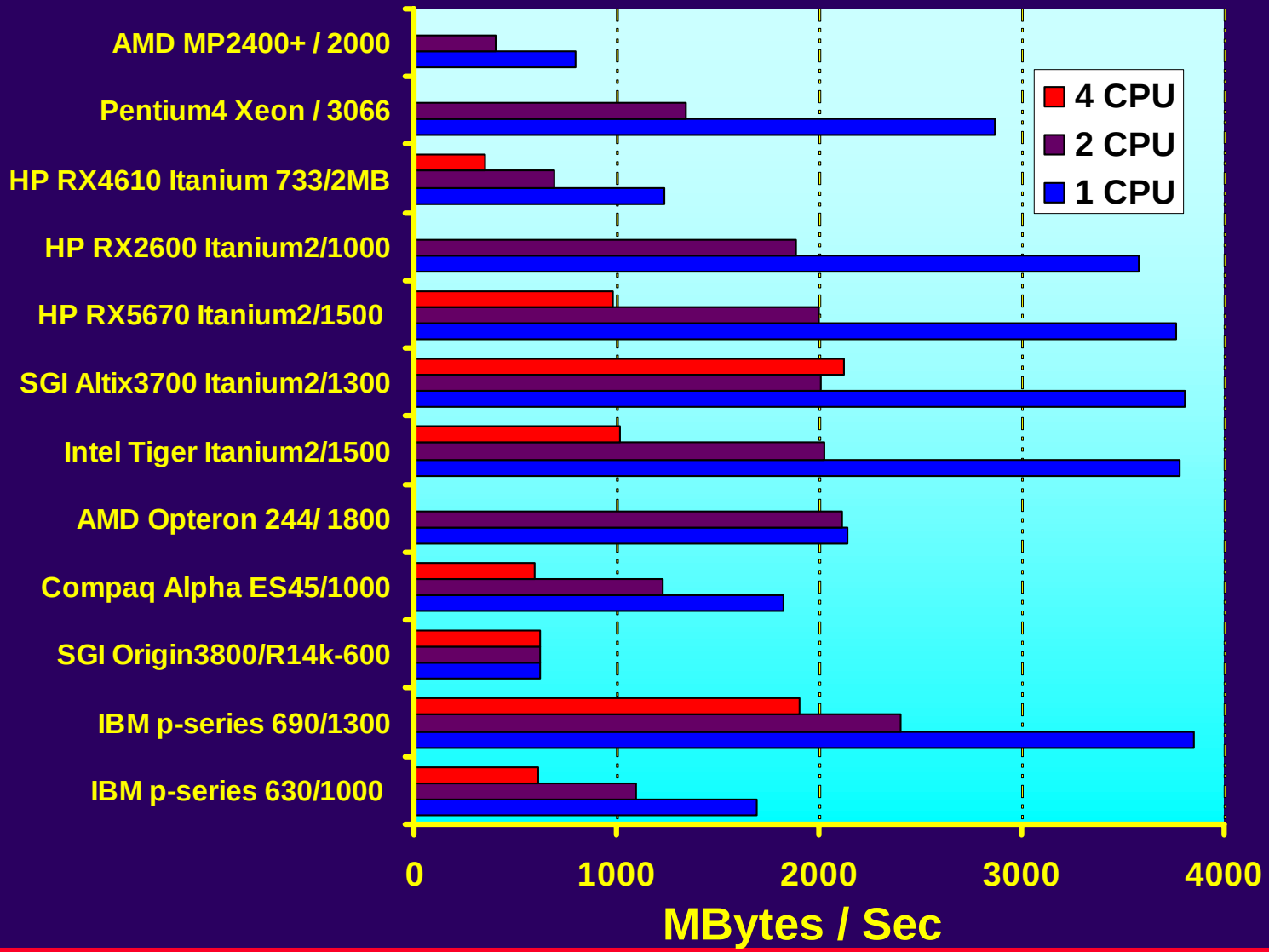
Performance relative to the IBM p-series 690/pwr4 1.3 GHz



STREAM: Measured Sustainable Memory Bandwidth in HPC (TRIAD)

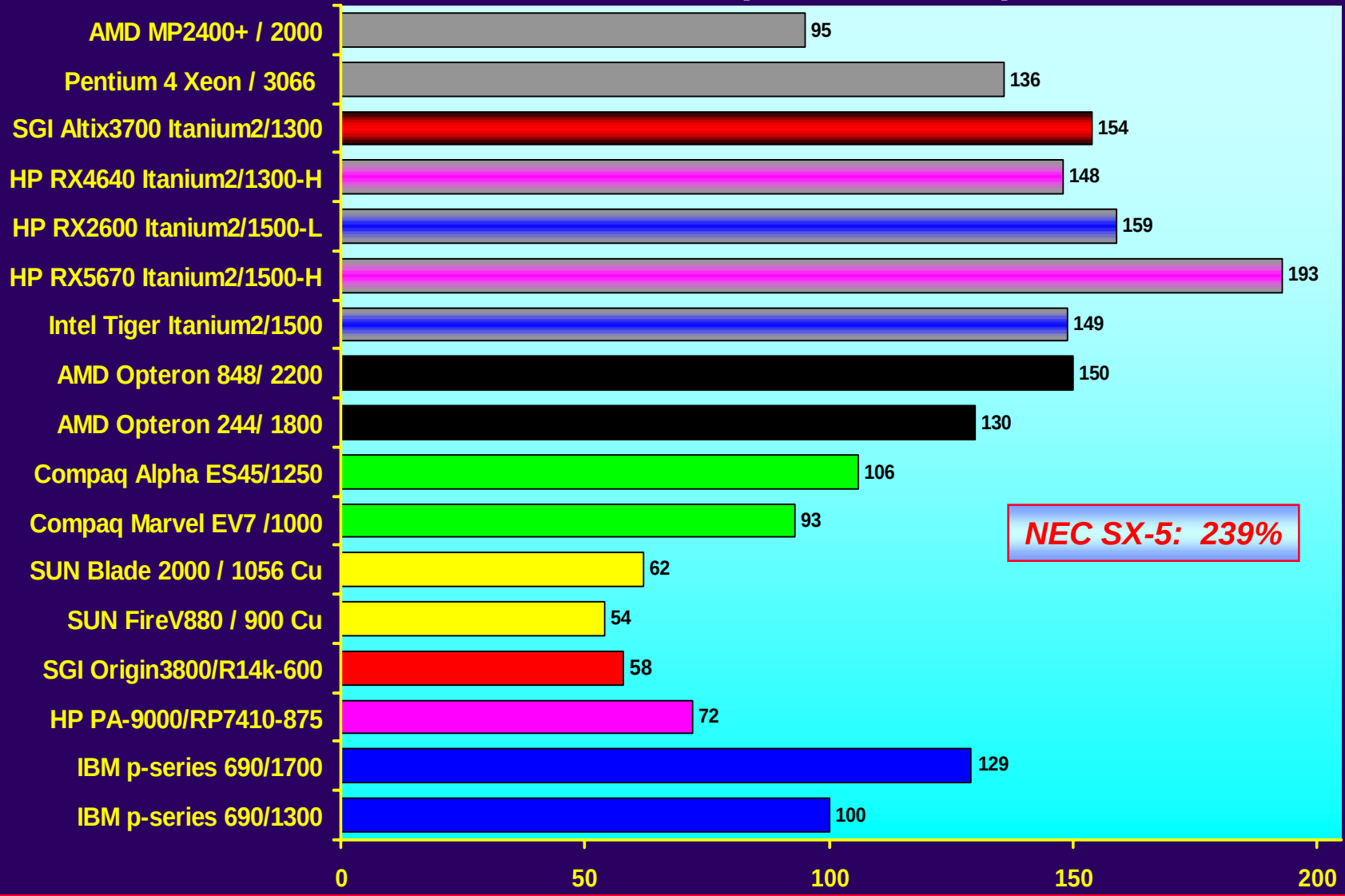


STREAM: Sustainable Memory Bandwidth (TRIAD) per process



Computational Chemistry Kernels.

Performance relative to the IBM p-series 690/pwr4 1.3 GHz



GAMESS-UK and DL_POLY Benchmarks

GAMESS-UK

12 Typical QC Calculations

Module	Basis (GTOs)	Species
1. SCF	STO-3G (124)	Morphine
2. SCF	6-31G (154)	$C_6H_3(NO_2)_3$
3. ECP Geometry	ECPDZ (70)	Na_7Mg^+
4. Direct-SCF	6-31G (82)	Cytosine
5. CAS-geometry	TZVP (52)	H_2CO
6. MCSCF	EXT1 (74)	H_2CO
7. Direct-CI	EXT2 (64)	H_2CO/H_2+CO
8. MRD-CI (26M)	ECP (59)	$TiCl_4$
9. MP2-geometry	6-31G* (70)	H_3SiNCO
10. SCF 2nd derivs.	6-31G (64)	C_5H_5N
11. MP2 2nd derivs.	6-31G* (60)	C_4
12. Direct-MP2	DZP (76)	C_5H_5N

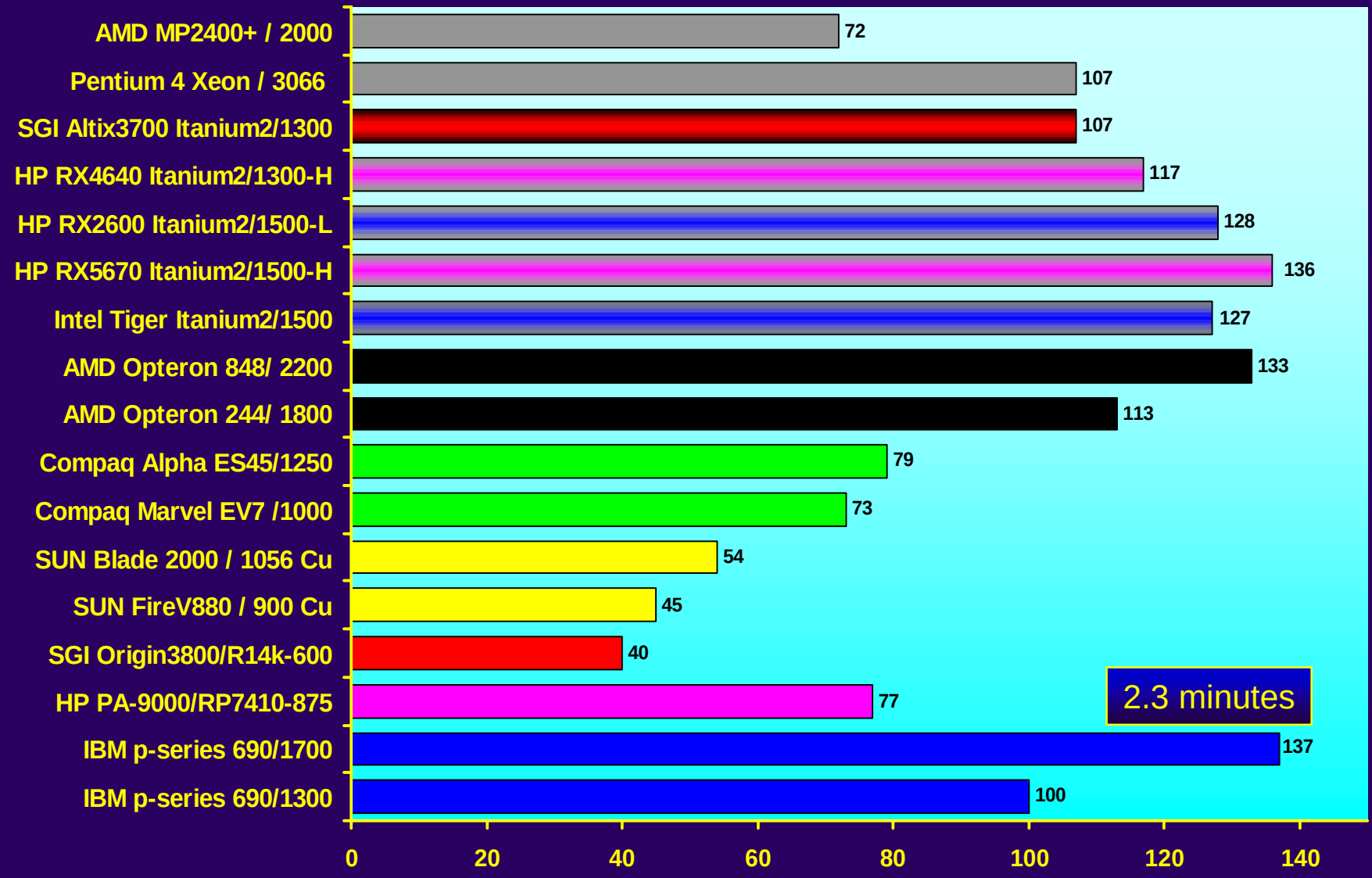
DL_POLY

Six Typical Simulations

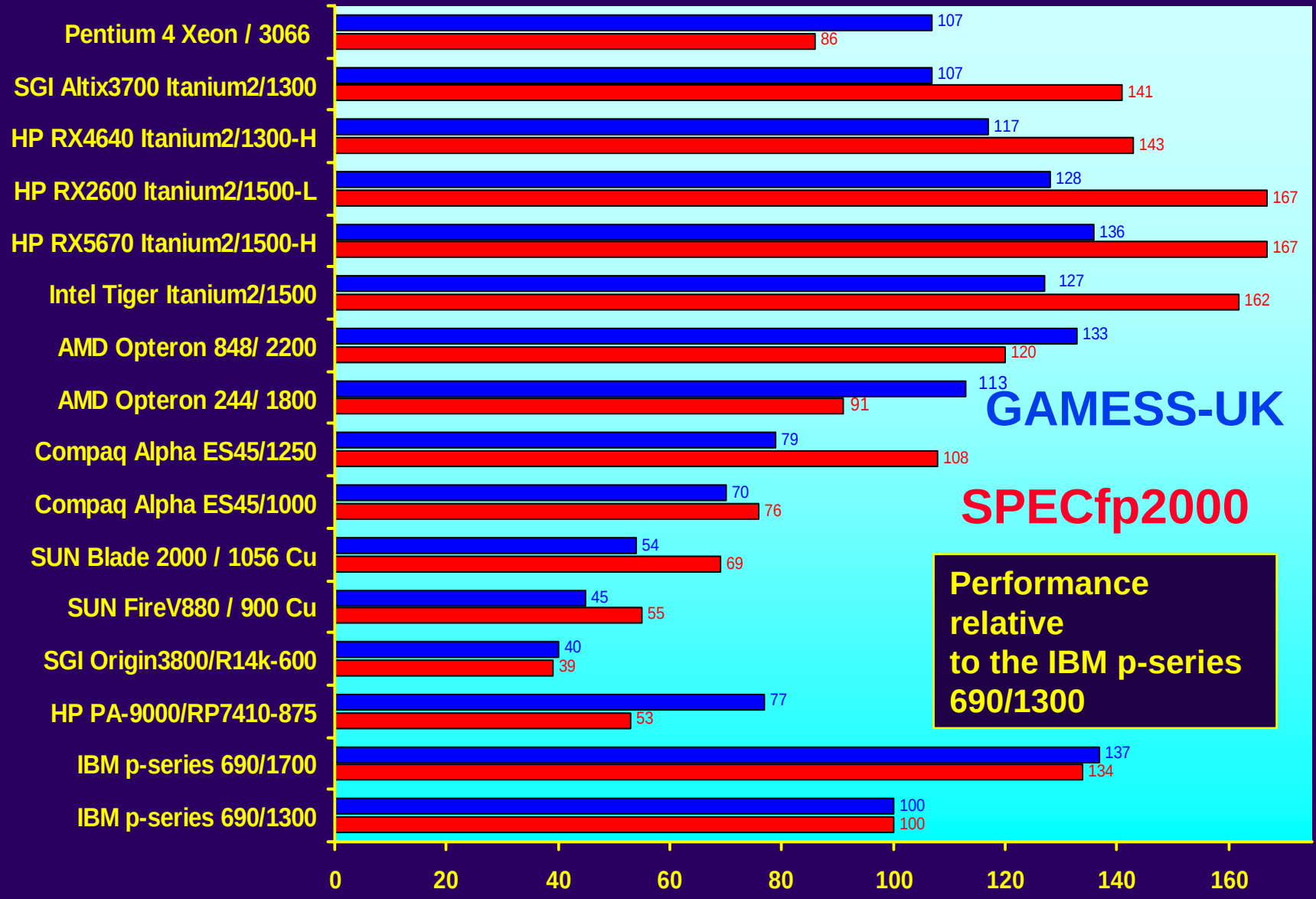
Simulation	Atoms	Time steps
1. Na-K disilicate glass	1080	300
2. Metallic Al with Sutton-Chen potential	256	8000
3. Valinomycin in 1223 water molecules	3837	100
4. Dynamic shell model water with 1024 sites	768	1000
5. Dynamic shell model MgCl2 with 1280 sites	768	1000
6. Model membrane, 2 membrane chains, 202 solute and 2746 solvent molecules	3148	1000

The GAMESS-UK Benchmark I. CPU

Performance relative to the IBM p-series 690/pwr4 1.3 GHz



SPECfp2000 and the GAMESS-UK Benchmark



The GAMESS-UK-99 Benchmark

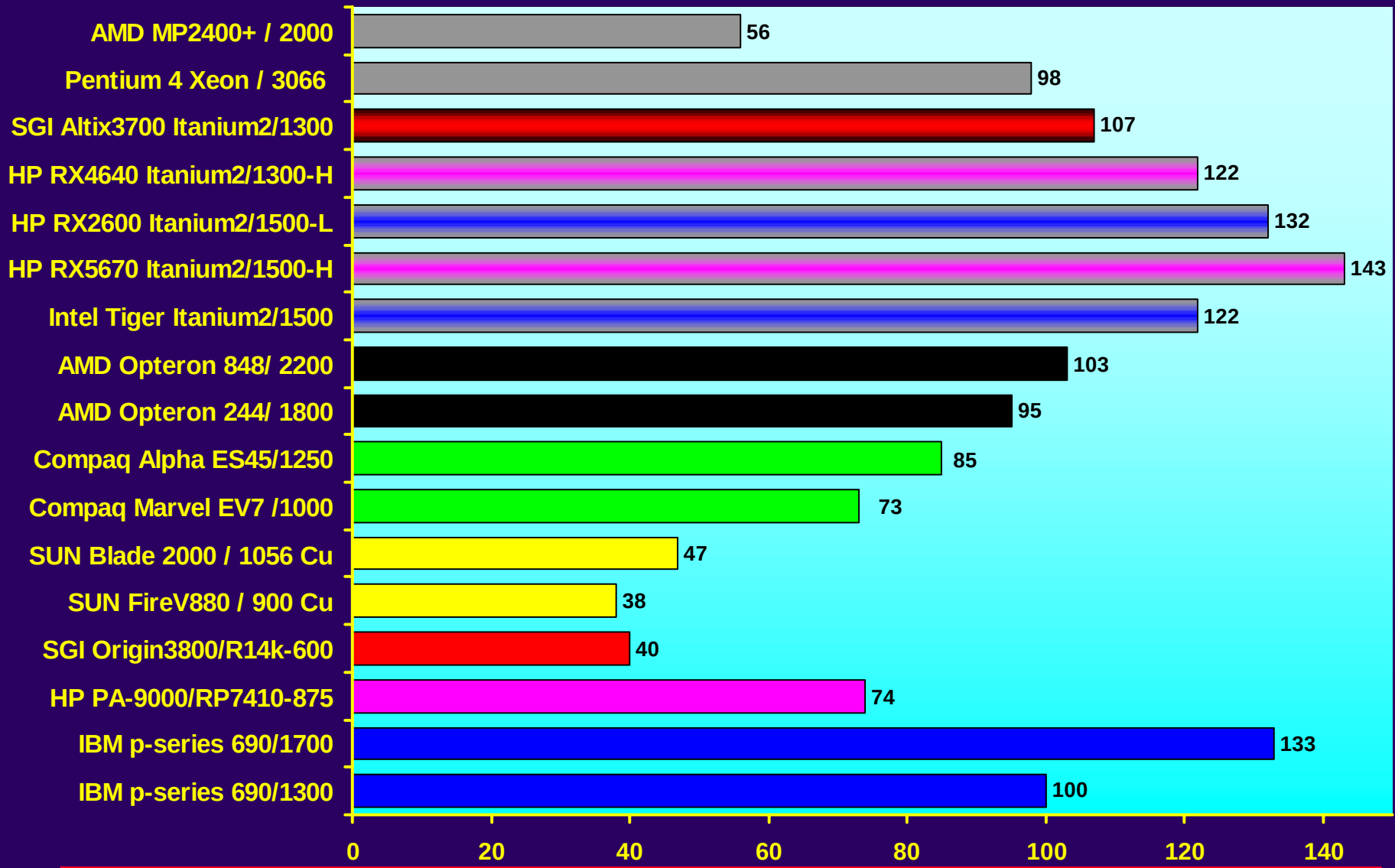
10 Typical QC Calculations

Module	Basis (GTOs)	Species
1. Direct- SCF	6-31G (227)	Morphine
2. SCF	6-31G** (265)	$C_6H_3(NO_2)_3$
3. DFT B3LYP	6-311G* (167)	Cytosine
4. MCSCF	CC-PVTZ (100)	H_2CO
5. Direct-CI	CC-PVTZ (100)	H_2CO/H_2+CO
6. CCSD(T)	TZV+2d+1f (144)	C_4
7. MP2-geometry	TZVP (105)	H_3SiNCO
8. SCF 2nd derivs.	6-311G** (144)	C_5H_5N
9. MP2 2nd derivs.	TZVP(C2d) (104)	C_4
10. Direct-MP2	6-31G* (130)	Cytosine

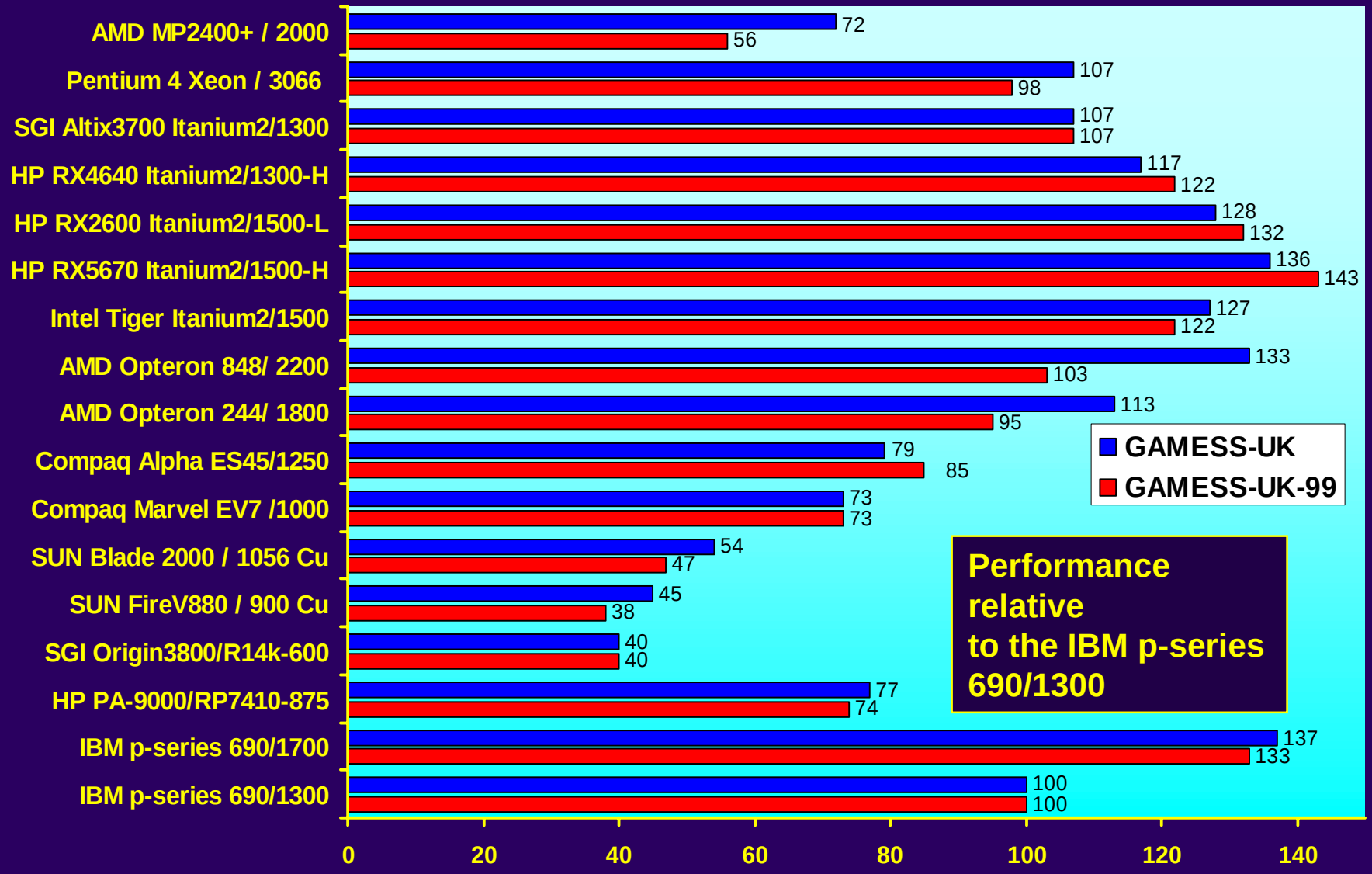
Benchmark Time: 30.8 minutes on **IBM p-series 690/pwr4 1.3 GHz**

The GAMESS-UK-99 Benchmark

Performance relative to the IBM p-series 690/pwr4 1.3 GHz

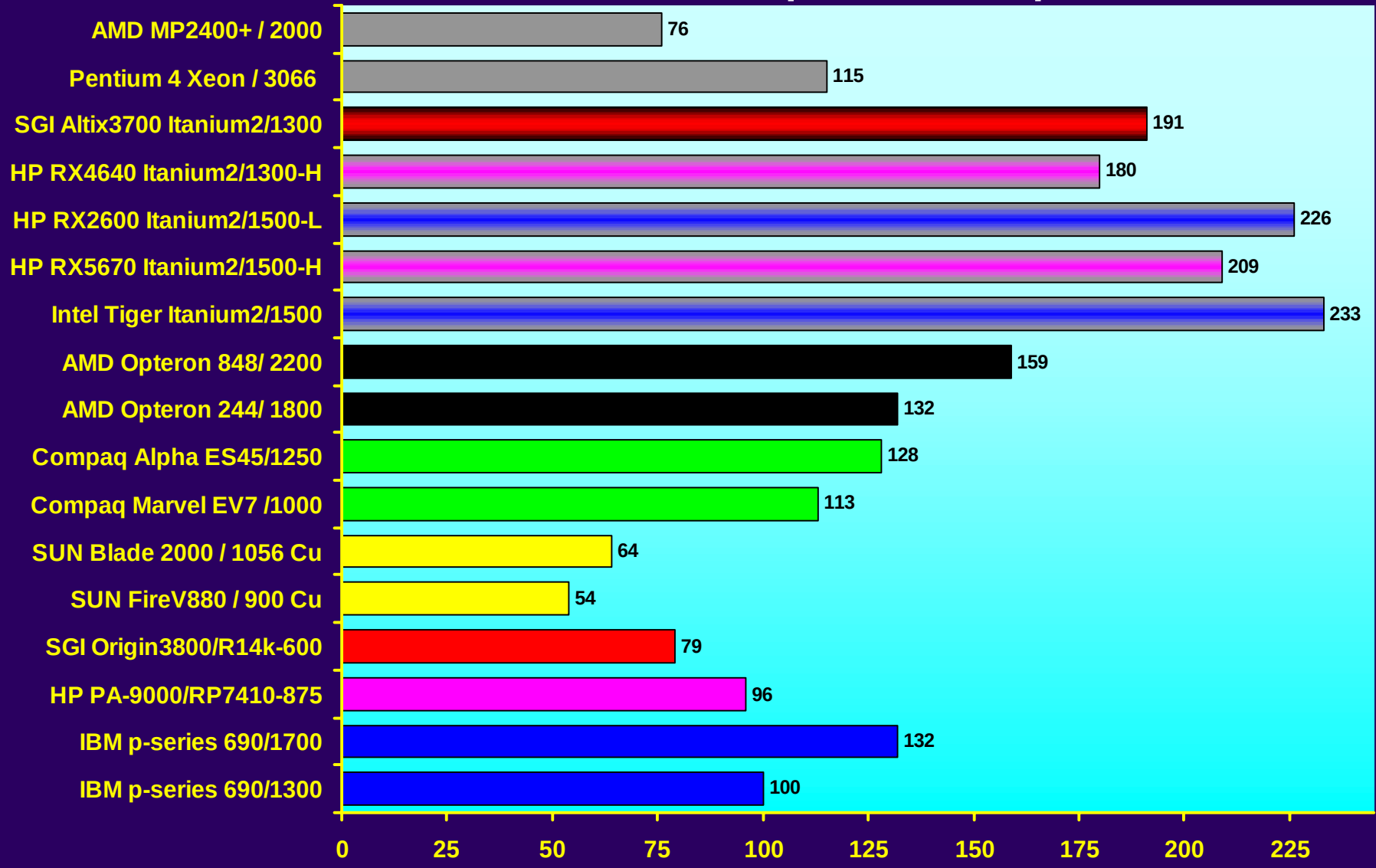


The GAMESS-UK and GAMESS-UK-99 Benchmark

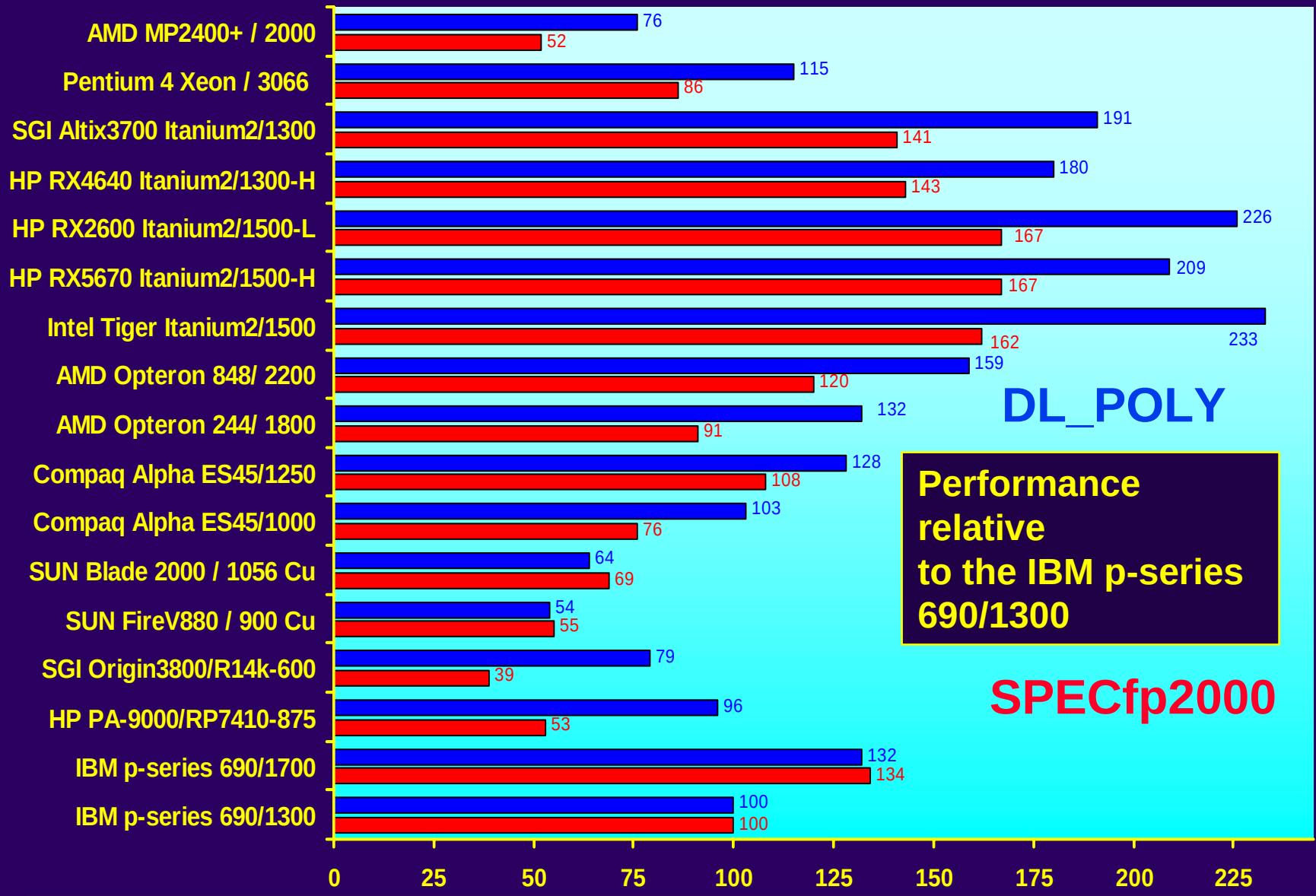


The DL_POLY Benchmark.

Performance relative to the IBM p-series 690/pwr4 1.3 GHz

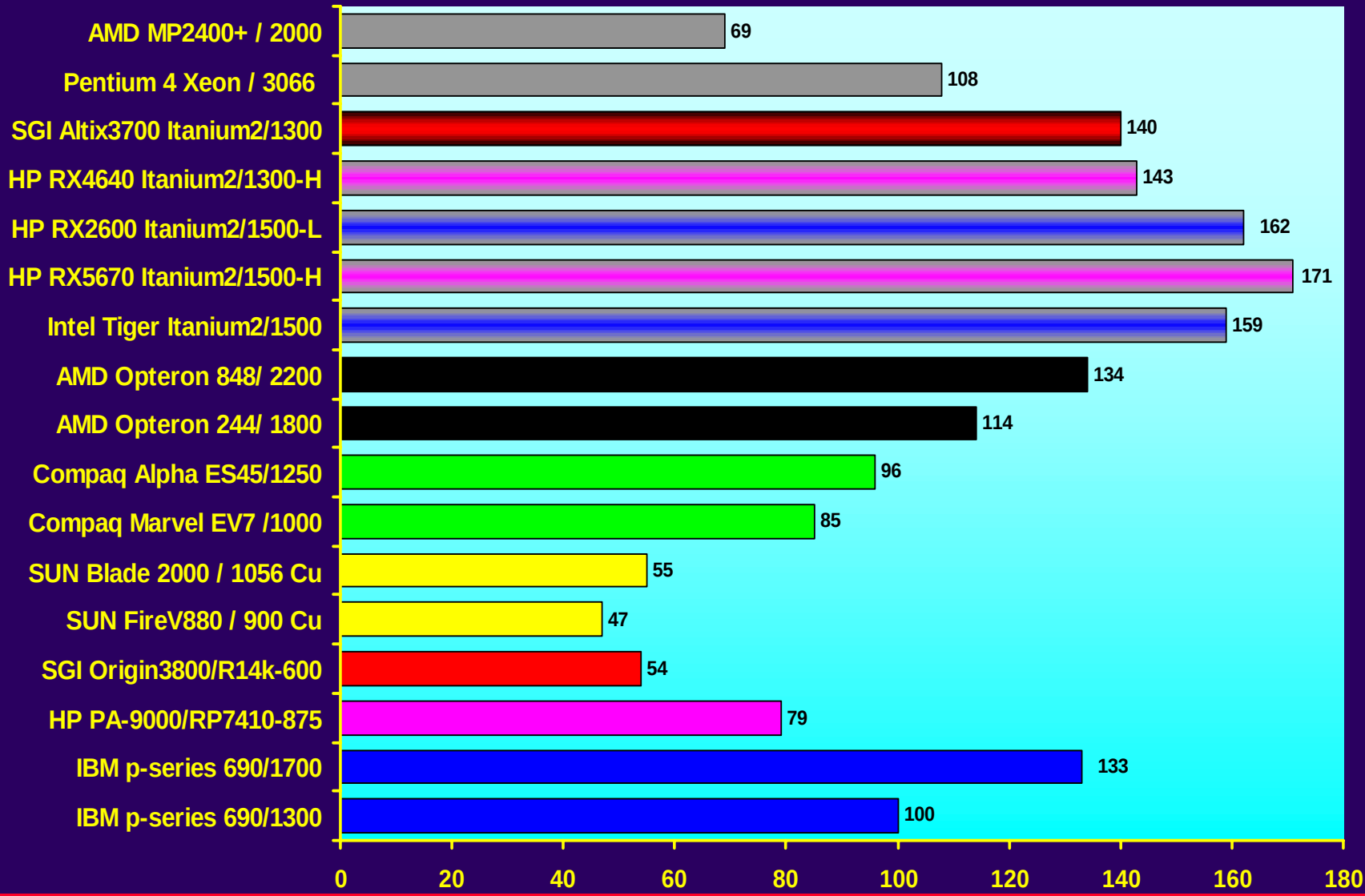


SPECfp2000 and the DL_POLY Benchmark



Summary Index relative to the IBM p-series 690/pwr4 1.3 GHz

The MATRIX-97, Chemistry Kernels, GAMESS-UK and DLPOLY Benchmarks



Computational Chemistry Rate Benchmark

- "Rate" Benchmark suite recently developed to incorporate:
  - Matrix "kernels" (MATRIX-97+)
  - Application packages (e.g. GAMESS-UK-99, DL_POLY+)
- Multi-component benchmark:
  - Matrix Operations / Matrix multiplication and matrix diagonalisation
  - Quantum Chemistry Calculations
  - Molecular Dynamics Calculations
- Rate Procedure:
  - For each benchmark (i) run *n* instances at once and take elapsed time (last to finish - first to start).
  - The rate for this benchmark is R_i = *n* X T_ref / T_i
  - T_ref is the elapsed time on a reference system. (IBM p-series 690/pwr4 1.3 GHz scaled to a single processor (*n*=1) elapsed time of 100 units)
  - Take "the geometric mean" of all the benchmarks (with the same *n*).

Components of Chemistry Rate Benchmark

1. MATRIX OPERATIONS (MATRIX-97+)

- SPARSE Matrix Multiply BenchMark: Vector FORTRAN and DGEMM
  - series of MMOs (R = A X B) are performed involving matrices of increasing order:
    - MATRIX-97+: 100, 200, … , 1200 (B is sparse)

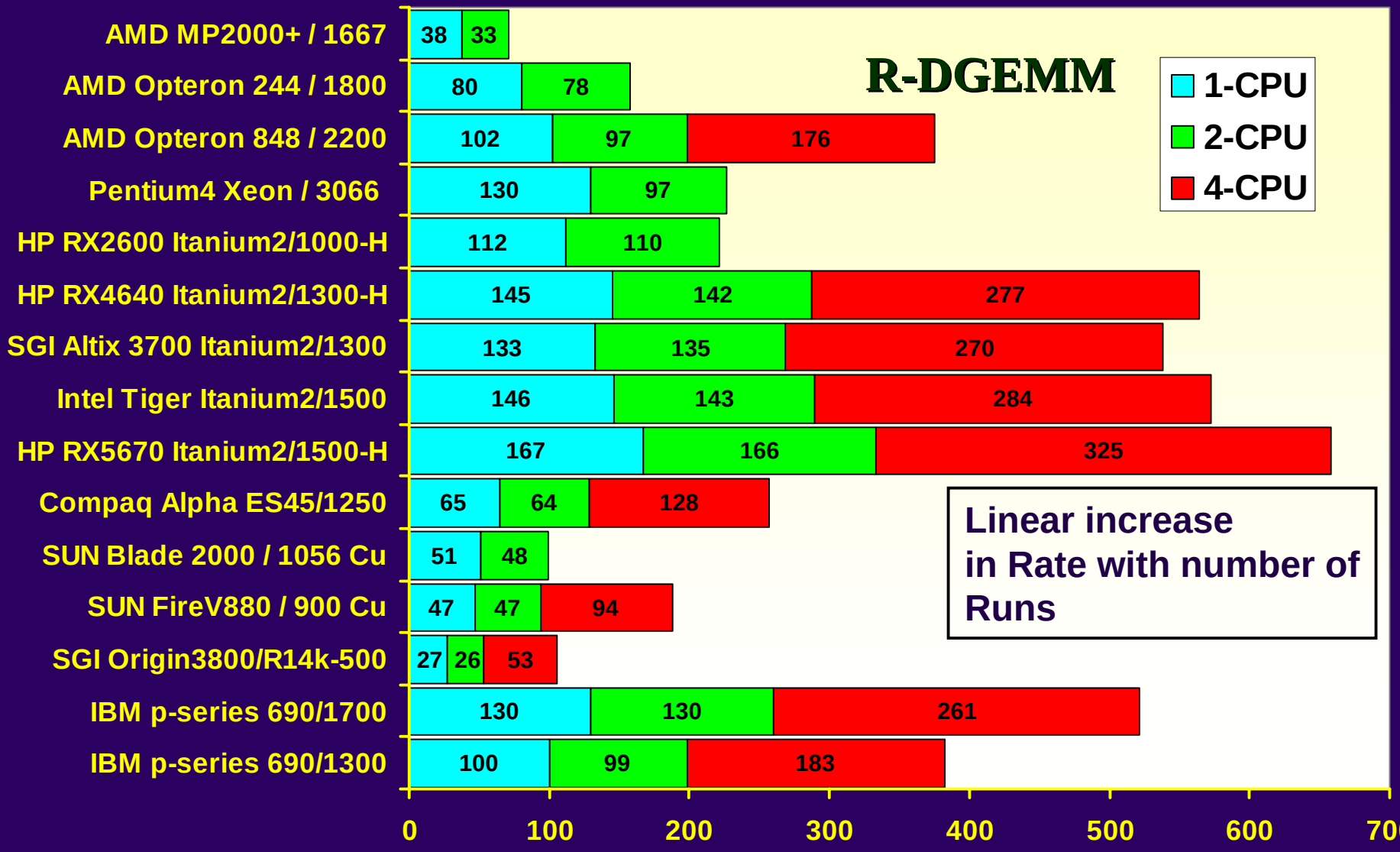
Memory bandwidth

- Diagonalisation Benchmark
  - performance of 7 routines from mathematical libraries and QC codes:
    - MATRIX-97+: 100, 200, …, 600
- $Q^{\dagger}HQ$ Benchmark
  - involves use of library routines e.g. BLAS. Uses both a scalar and vector algorithm (DGEMM):
    - MATRIX-97+: 100, 200, … , 1000

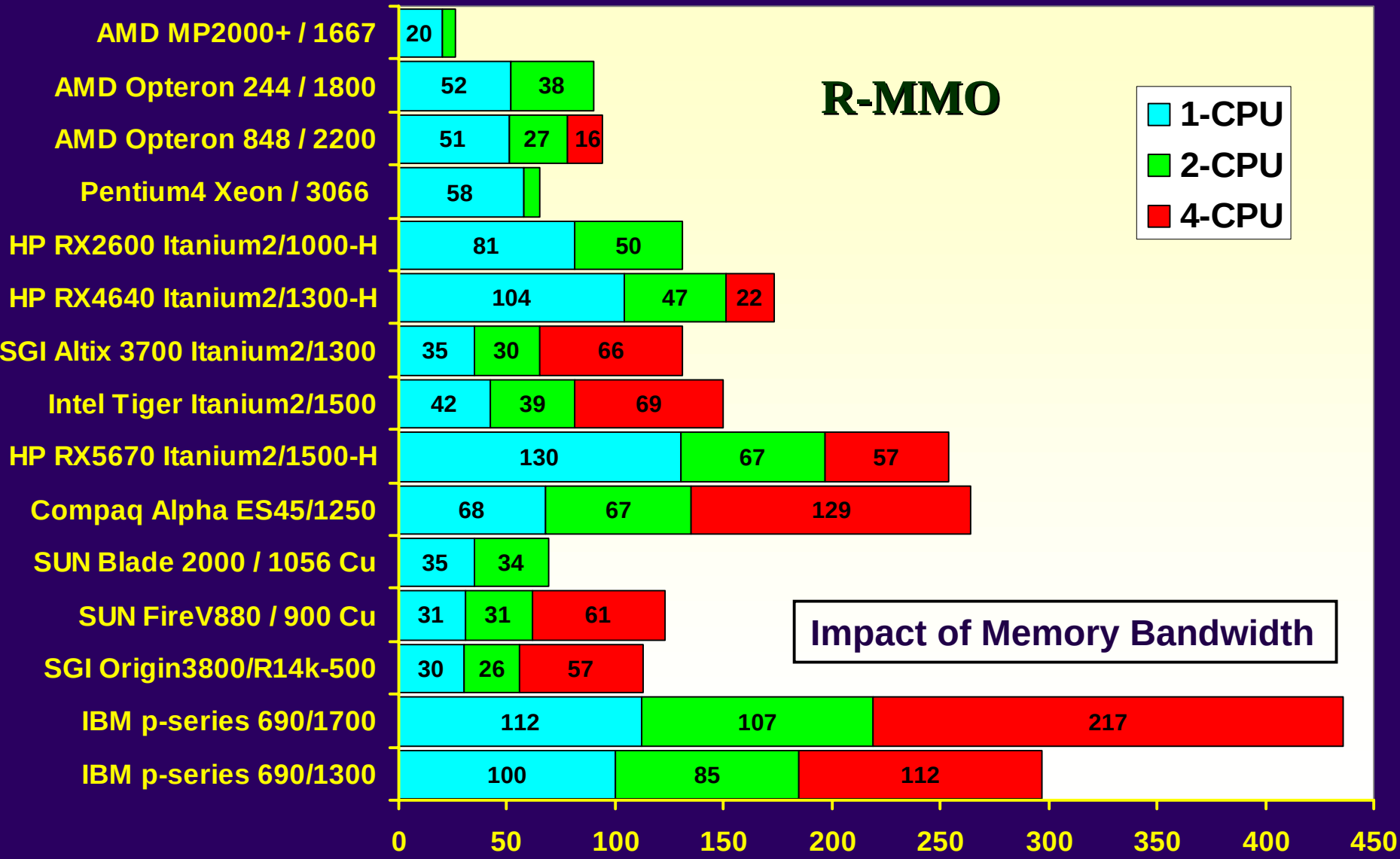
-lblas

2. DLPOLY
   - 5 simulations (increased no. of time steps)
3. GAMESS-UK
   - 8 Calculations (GAMESS_UK-99 : Direct- SCF, DFT B3LYP, MCSCF, Direct-CI, MP2-geometry, SCF 2^{nd} derivs., MP2 2^{nd} derivs., Direct-MP2)

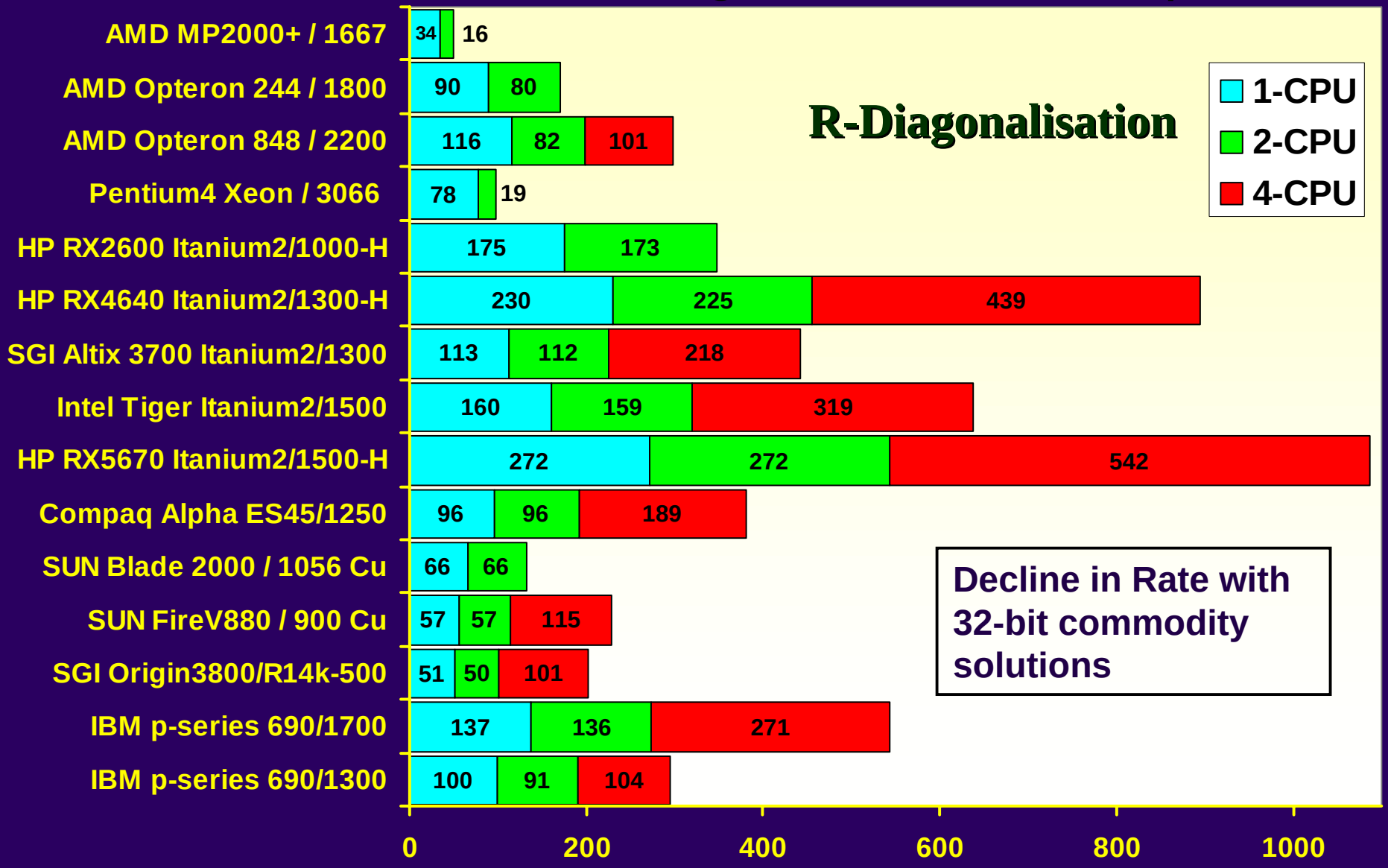
Rate Benchmark: DGEMM Component



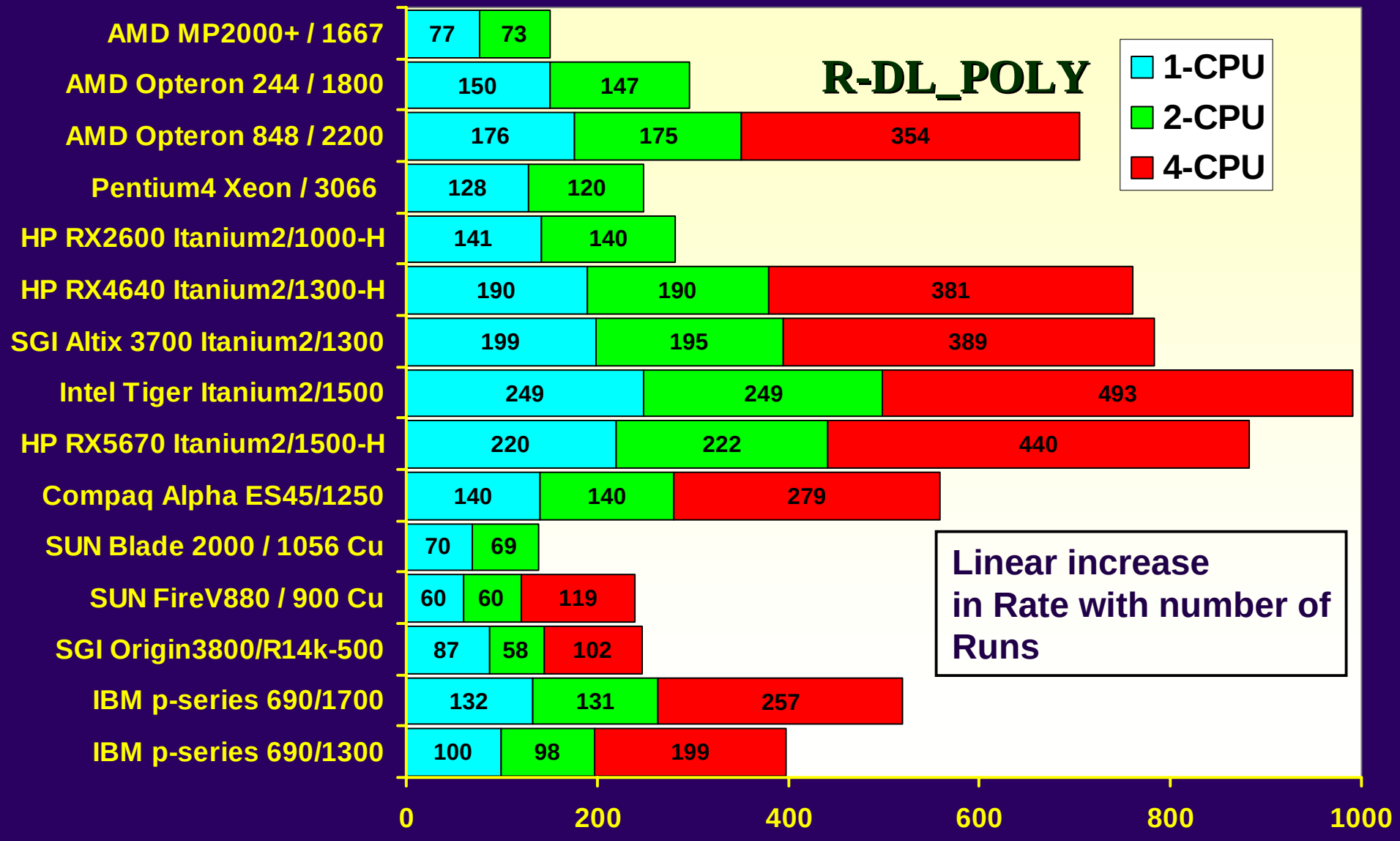
Rate Benchmark: MMO FORTRAN



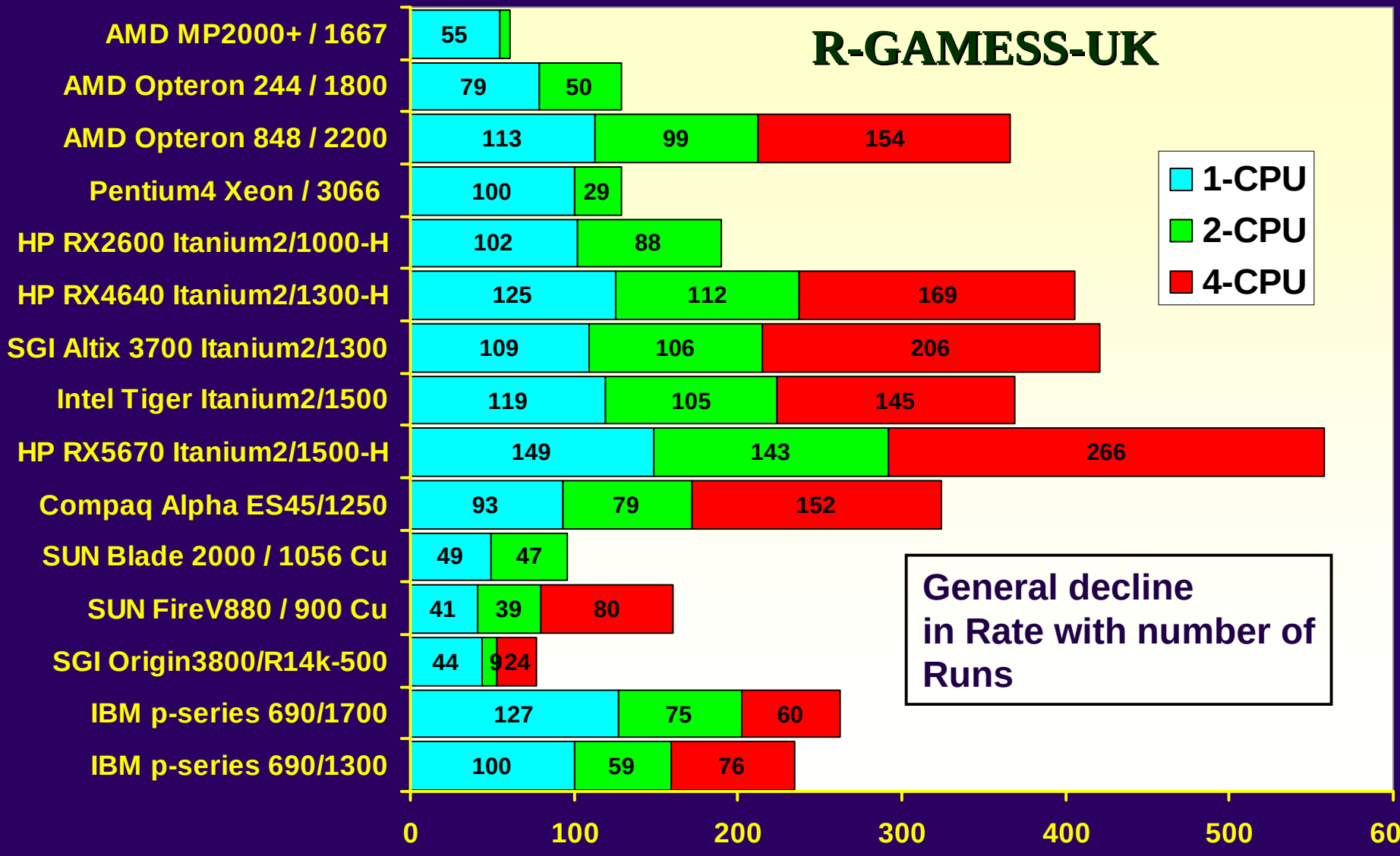
Rate Benchmark: Diagonalisation Component



Rate Benchmark: DL_POLY Component



Rate Benchmark: GAMESS-UK Component



Computational Chemistry Rate Metric

- Chemistry Rate Metric:
  - For each component benchmark (i) run *n* instances at once and take elapsed time (last to finish - first to start).
  - Component rate R_i = *n* X T_ref / T_i
  - T_ref is the elapsed time on the IBM p-series 690/pwr4 1.3 GHz scaled to a single CPU time of 100 units.

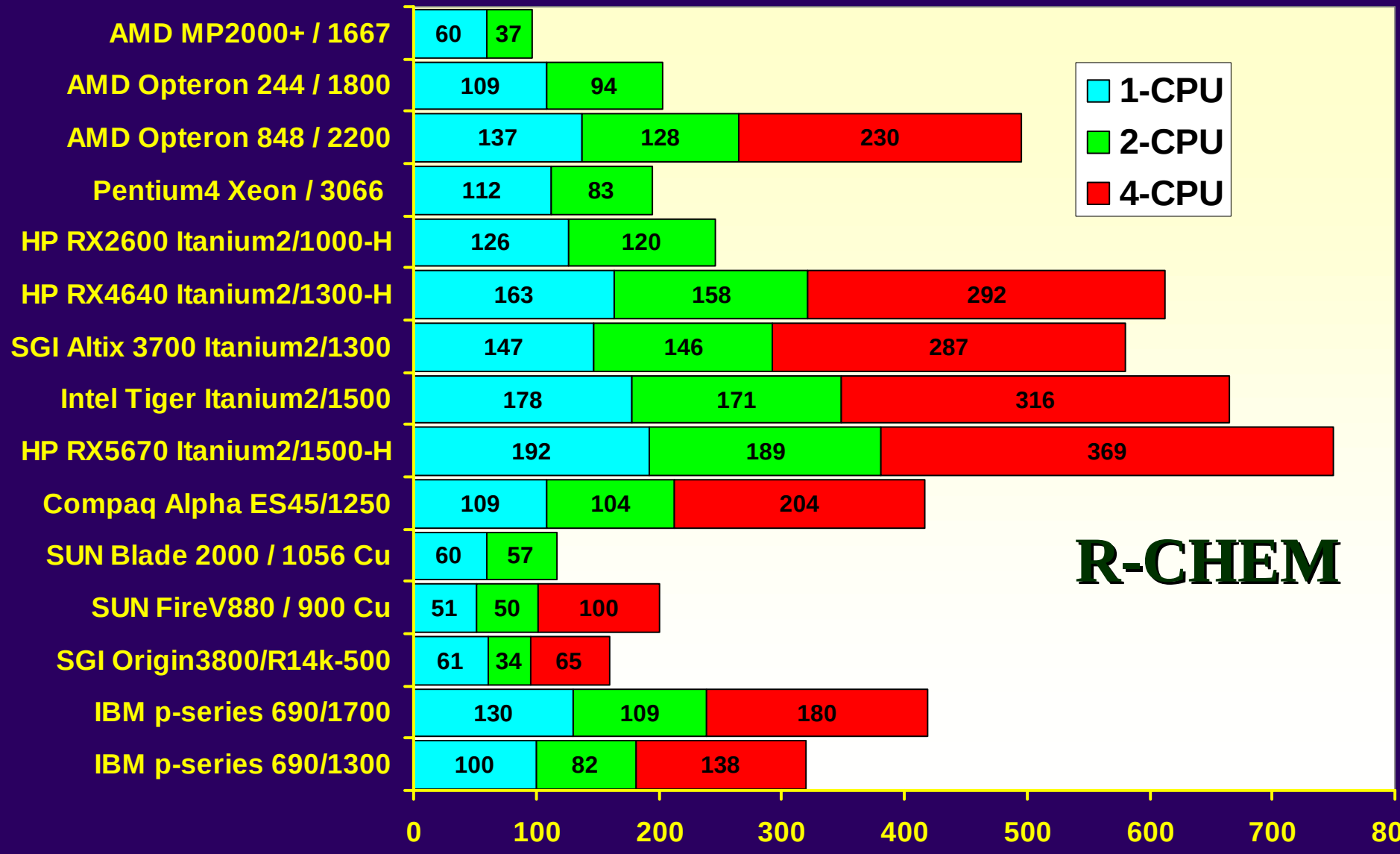
R_*CHEM* = *0.1* X R_***DGEMM*** +

0.1 X R_***Diagonalisation*** +

0.4 X R_*DLPOLY* +

0.4 X R_*GAMESS-UK*

Chemistry Rate Benchmark



Evaluation and Benchmarking of High-end and Commodity-based Sytems

Parallel Systems and Capacity Computing

High-End Systems Evaluated

- Cray T3E/1200E
  - 816 processor system at Manchester (CSAR), 600 Mz Alpha EV56 CPU, 256 MB
- IBM SP/WH2-375 and *SP/p690*
  - 32 CPU system at DL, 4-way WH2 SMP "thin nodes" with 2 GB memory, 375 MHz Power3-II processors with 8 MB L2 cache
  - **IBM Regatta-H** (32-way node, 1.3 GHZ power4 CPUs) at Montepelier
  - ***IBM SP/p690* (8-way LPAR'd nodes, 1.3 GHZ) at Daresbury (1280 CPUs, HPCx)**
- Compaq AlphaServer SC
  - 4-way ES40/667 A21264A (APAC) and 833 MHz SMP nodes (2 GB RAM);
  - ***TCS1 system at PSC*** (comprising 750 4-way ES45 nodes - 3,000 EV68 CPUs - with 4 GB memory per node, 8MB L2 cache)
  - Quadrics "fat tree" interconnect (5 usec latency, 250 MB/sec B/W)
- SGI Origin 3800
  - SARA (1000 CPUs) - Numalink with MIPS R14k/500 CPUs
- *SGI Altix 3700*
  - ***Linux Cluster - Numalink with Itanium 2 1.3 GHz CPUs, 3MB L3 cache***
  - ***CSAR ("newton" 256 CPUs) and SARA ("aster" - 416 CPUs - 7 nodes)***

Commodity Systems (CSx)
Prototype / Evaluation Hardware

Systems	Location	CPUs	Configuration
CS1	Daresbury	32	PentiumIII / 450 MHz + FE (EPSRC)
CS2	Daresbury	64	24 X dual UP2000/EV67-667, QSNet Alpha/LINUX cluster, 8 X dual CS20/EV67-833 (“loki”)
CS3	RAL	16	Athlon K7 850MHz + myrinet
CS4	*Sara*	32	Athlon K7 1.2 GHz + FE
CS6	*CLiC*	528	PentiumIII / 800 MHz; fast ethernet (Chemnitzer Cluster)
CS7	Daresbury	64	AMD K7/1000 MP + SCALI/SCI (“ukcp”)
CS8	*NCSA*	320	160 dual IBM Itanium/800 + Myrinet 2k (“titan”)
CS9	*Bristol*	96	Pentium4 Xeon/2000 + Myrinet 2k (“dirac”)
Protoype Systems			
CS0	Daresbury	10	10 CPUS, Pentium II/266
CS5	Daresbury	16	8 X dual Pentium III/933, SCALI

www.cse.clrc.ac.uk/Activity/DisCo

Commodity Systems (CSx) II.
Evaluation Hardware

Systems	Location	CPUs	Configuration
CS10	*Hull*	64	Pentium4 Xeon/2666 + Myrinet 2k ("eagle"), Streamline/SCORE
CS11	*Workstations UK*	32	Pentium4 Xeon/2400 + GbitEther, ScaMPI
CS12	*Essex*	48	Pentium4 Xeon/2400 + GbitEther ("sstream1"), Streamline/SCORE
CS13	*White Rose, Leeds*	256	Pentium4 Xeon/2200-2400 + Myrinet 2k, ("snowdon"), Streamline/SCORE
CS14	*NCSA*	1024	Pentium III Xeon/1000 + Myrinet 2k ("platinum")
CS15	*SDSC*	128	Pentium III Xeon/ 8000 + Myrinet 2k ("meteor")
CS16	*SDSC*	256	dual-Itanium2/1.3 GHz nodes + Myrinet 2k ("Teragrid")

Applications Performance Overview

- ***Serial (SPEC, DL) & Communication Benchmarks***
- ***Parallel Applications Performance***

1. Computational Chemistry: Molecular Simulation & Electronic Structure
2. Computational Materials Science
3. Atomic & Molecular Physics
4. Computational Engineering
5. Environmental Modelling

- Capacity-based group solution
- Issues of Cost effectiveness
- On e.g. 128-256 CPU cluster, modal job size is ~ 32 CPUs
- Increasing trend to hierarchical clusters - Gbit network with HEC core (with e.g. myrinet)

Capability and Capacity Computing
Commodity vs. Proprietary Solutions

Performance Metrics: 1999-2001

Attempted to quantify delivered performance from the Commodity-based systems against current MPP (CSAR Cray T3E/1200E)and ASCI-style SMP-node platforms (e.g. SGI Origin 3800) i.e.

Performance Metric (% 32-node Cray T3E)

T (32-nodes Cray T3E/1200E) / T (32 CPUs) CSx

[$T_{32\text{-node}}$ *T3E* / $T_{32\text{-node}}$ *CS1 Pentium III/450 + FE*]

$T_{32\text{-node}}$ **T3E /** $T_{32\text{-node}}$ **CS6 Pentium III/800 + FE**

$T_{32\text{-node}}$ **T3E /** $T_{32\text{-CPU}}$ **CS2 Alpha Linux Cluster + Quadrix**

Performance Metrics: 2002

Performance Metric (% 32-node AlphaServer SC [PSC])

T (32-CPUs AlphaServer SC ES45/1000) / T (32 CPUs) CSx

$T_{32\text{-CPU}}$ **AlphaServer ES45 /** $T_{32\text{-CPU}}$ **CS9 Pentium 4 Xeon / 2000 + Myrinet 2k**

Commodity Comparisons with High-end Systems:
Compaq AlphaServer SC ES45/1000 and the SGI O3800/R14k-500

CS9 - Pentium4/2000 Xeon + Myrinet 2k

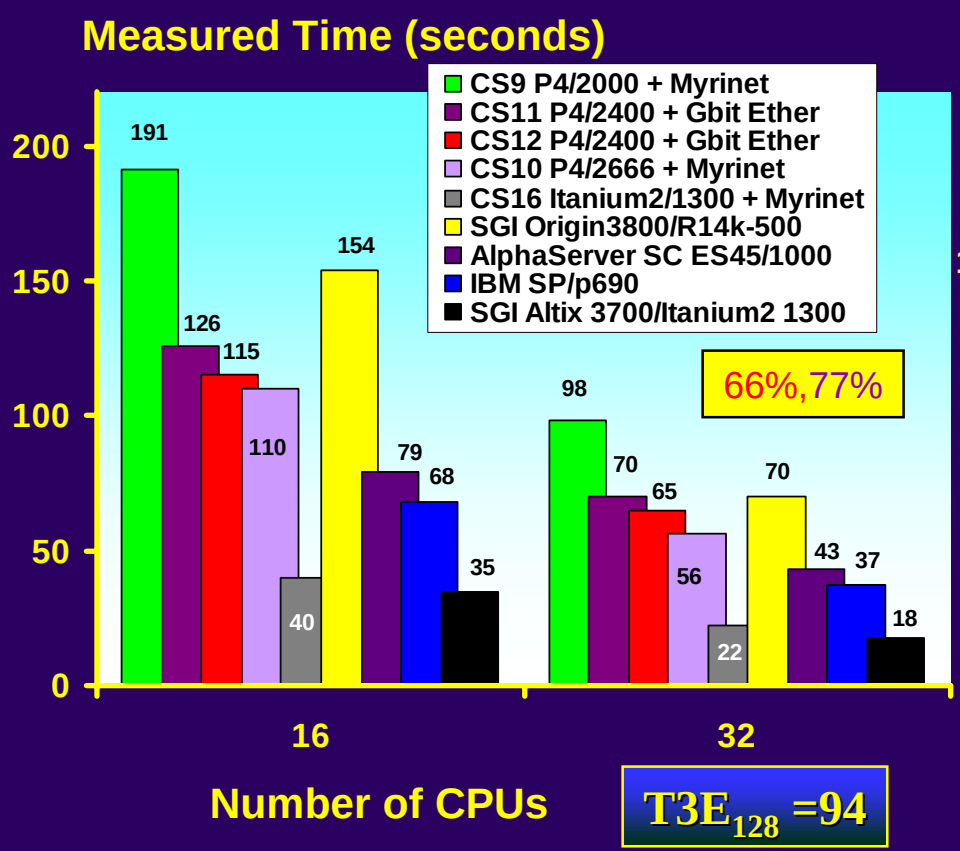
2002

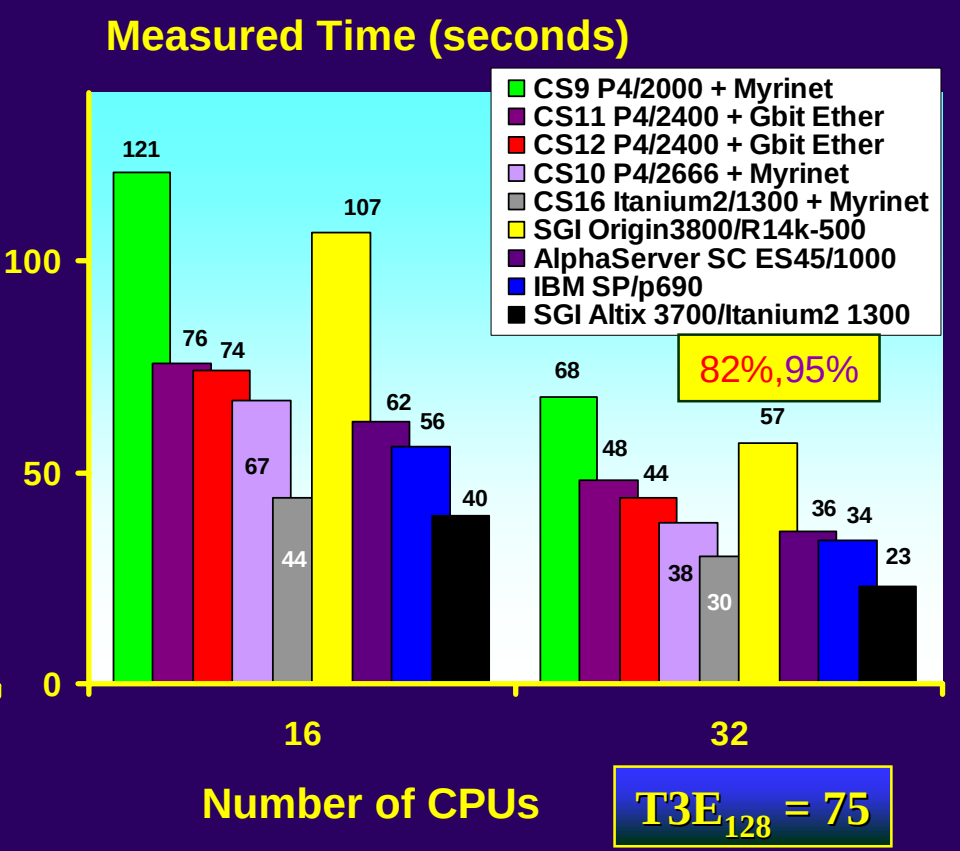
% of 32-CPU	AlphaServer SC	Origin 3800
GAMESS-UK		
SCF	**95%**	**135%**
DFT	**70-73%**	**117-161%**
DFT (Jfit)	**59-70%**	**92-111%**
DFT Gradient	**69%**	**114%**
MP2 Gradient	**59%**	**78%**
SCF Forces	**92%**	**148%**
NWChem (DFT Jfit)	**65-88%**	**94-227%**
GAMESS / CHARMM	**89%**	**139%**
DL_POLY		
Ewald-based	**44-53%**	**71-84%**
bond constraints	**41%**	**64%**
CHARMM	**95%**	**103%**
CASTEP	**47-67%**	**75-81%**
CPMD	**30%**	**53%**
ANGUS	**35-69%**	**51-147%**

DL_POLY V2: High-end and Commodity-based Systems

Bench 4. NaCl; 27,000 ions, Ewald , 75 time steps, Cutoff=24Å

Bench 5: NaK-disilicate glass; 8,640 atoms, MTS + Ewald: 270 time steps





Commodity Comparisons with High-end Systems: The Compaq AlphaServer SC ES45/1000

% of 32 CPUs of Compaq AlphaServer SC ES45/1000

Application	Cluster CS10 Pentium4/2666 Xeon + Myrinet 2k	CS12 Pentium4/2400 Xeon + Gbit Ethernet
GAMESS-UK		
SCF	**91%**	**85%**
DFT	**85-103%**	**78 - 95%**
DFT (Jfit)	**75%**	**70%**
DFT Gradient	**85%**	**85%**
MP2 Gradient	**59%** †	
SCF Forces	**92%** †	
DL_POLY- 2 (and - 3)		
Ionic Systems	**77- 95% (91%)**	**66-82% (84%)**
Macromolecular	**75% (92%)**	**61% (86%)**
CHARMM	**139%**	**104%**
CASTEP	**60-83%**	**53- 66%**
CPMD	**60-65%**	**55%**
ANGUS	**36-73%**	**34-72%**
SBLI	**53%**	**51%**

SUMMARY

- Processor Performance Overview
  - Single-processor performance, Performance Metrics
- SPECfp and Computational Chemistry Benchmark (serial)
  - Comparison involves 200+ computers
  - Matrix'89 and Matrix'97 kernels (MMO, diagonalisation), Application kernels" (SCF, MD, QMC and JACOBI + STREAM), Application packages (GAMESS-UK, DL_POLY)
- Increasing importance of Rate-based benchmarks:
  - SPECfp_rate and Chemistry Rate Benchmark
- Machine COSTS vs. Performance: URLs:
  - Powerpoint presentation and Paper:

    http://www.cse.clrc.ac.uk/disco/hw-perf.shtml
- Benchmarking & Evaluation of Commodity-based Systems
  - CS10 Xeon / 2666 cluster (Myrinet-2k) ca. 82% of Alpha ES45/1000.
  - Cost effectiveness of the CS12 Xeon / 2400 Cluster with Gbit Ethernet (Streamline, 75% of the Alpha ES45/1000).