

PERFORMANCE of VARIOUS COMPUTERS in COMPUTATIONAL CHEMISTRY

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CCLRC Daresbury Laboratory

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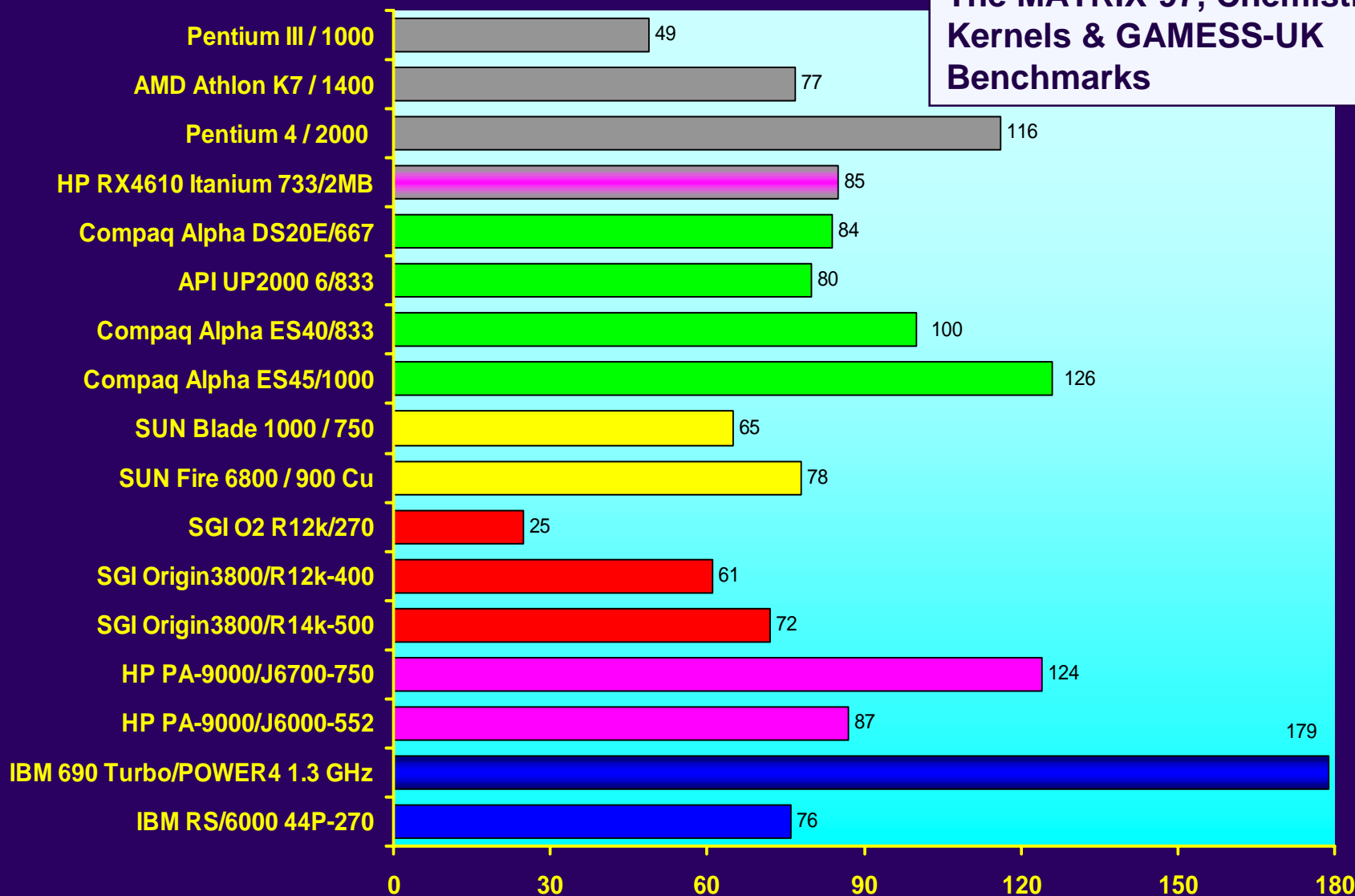
OUTLINE

- 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>

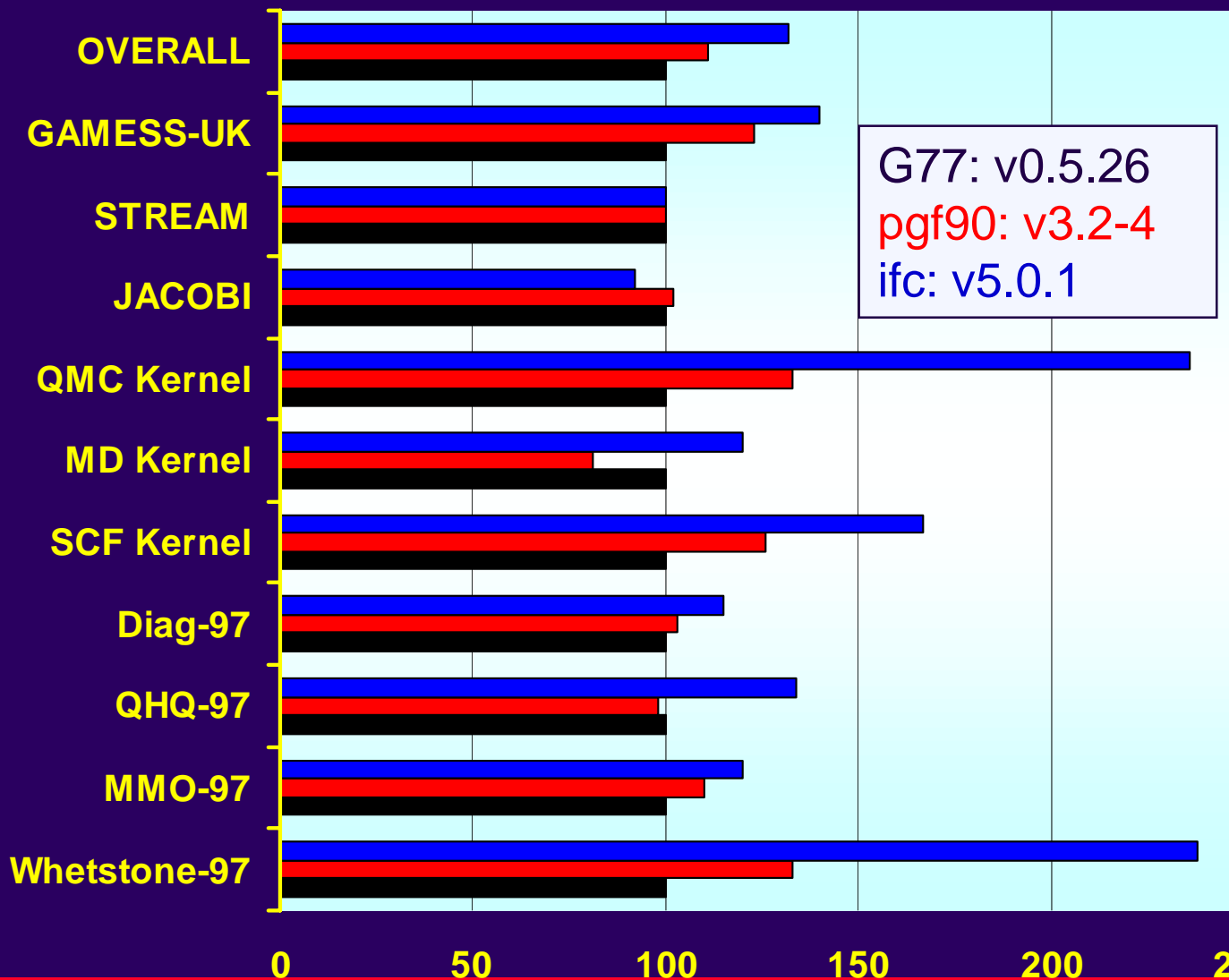
MEW12 (2001) - Summary PI relative to the Compaq Alpha ES40/833

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



Fortran Compilers - Performance

Performance relative to GNU g77 on Pentium 4/2000



MACHINES UNDER EVALUATION

<u>Machine</u>	<u>Processor</u>
<u>AMD Athlon</u> Pentium - PC	<u>MP 1.533 , 1.667 GHz, 2 GHz</u> Pentium 4- 1.5, 2.0 GHz
<u>SUN Blade 2000 / 1056 Cu</u> <u>SUN Fire V880 / 900 Cu</u>	<u>UltraSPARC-3 / 1056 MHz</u> <u>UltraSPARC-3 / 900 MHz</u>
<u>HP PA-9000 / J6700</u> <u>HP PA-9000 / RP7410</u>	<u>PA8700 / 750 MHz</u> <u>PA8700+ / 875MHz</u>
HP RX4610	Itanium / 733 MHz (2 MB L3)
<u>HP RX2600 (2-way)</u> <u>HP RX5670 (4-way)</u> <u>HP ZX6000</u>	<u>Itanium 2 / 1000 MHz (3 MB L3)</u> <u>Itanium 2 / 1000 MHz (3 MB L3)</u> <u>Itanium 2 / 900 MHz (1.5 MB L3)</u>
<u>Intel Tiger (4-way)</u>	<u>Itanium 2 / 1000 MHz (3 MB L3)</u>
<u>Compaq AlphaServer ES45</u> <u>Compaq AlphaServer ES45</u> <u>Compaq Alpha Marvel</u>	<u>AXP A21264C / 1000 MHz</u> <u>AXP A21264C / 1250 MHz</u> <u>EV7 1000 MHz</u>

<u>Machine</u>	<u>Processor</u>
<u>SGI Origin3800/R14k</u>	<u>R14000/R14010 600 MHz</u>
SGI Origin3800/R14k	R14000/R14010 500 MHz
SGI Origin300/R14k	R14000/R14010 500 MHz
SGI O2/R12k-SC	R12000/R12010 270 MHz
<u>IBM p-Series 630</u>	<u>RS/6000 /POWER4 1.0GHz</u>
<u>IBM p-Series 690</u>	<u>RS/6000 /POWER4 1.3GHz</u>
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
RS/6000 NH - 222 MHz

SPEC Benchmarks

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

NOT:

- Graphics
- Network
- I/O

<http://www.specbench.org>

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

- SPECratio - $T(\text{measured system}) / T(\text{reference})$
- 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

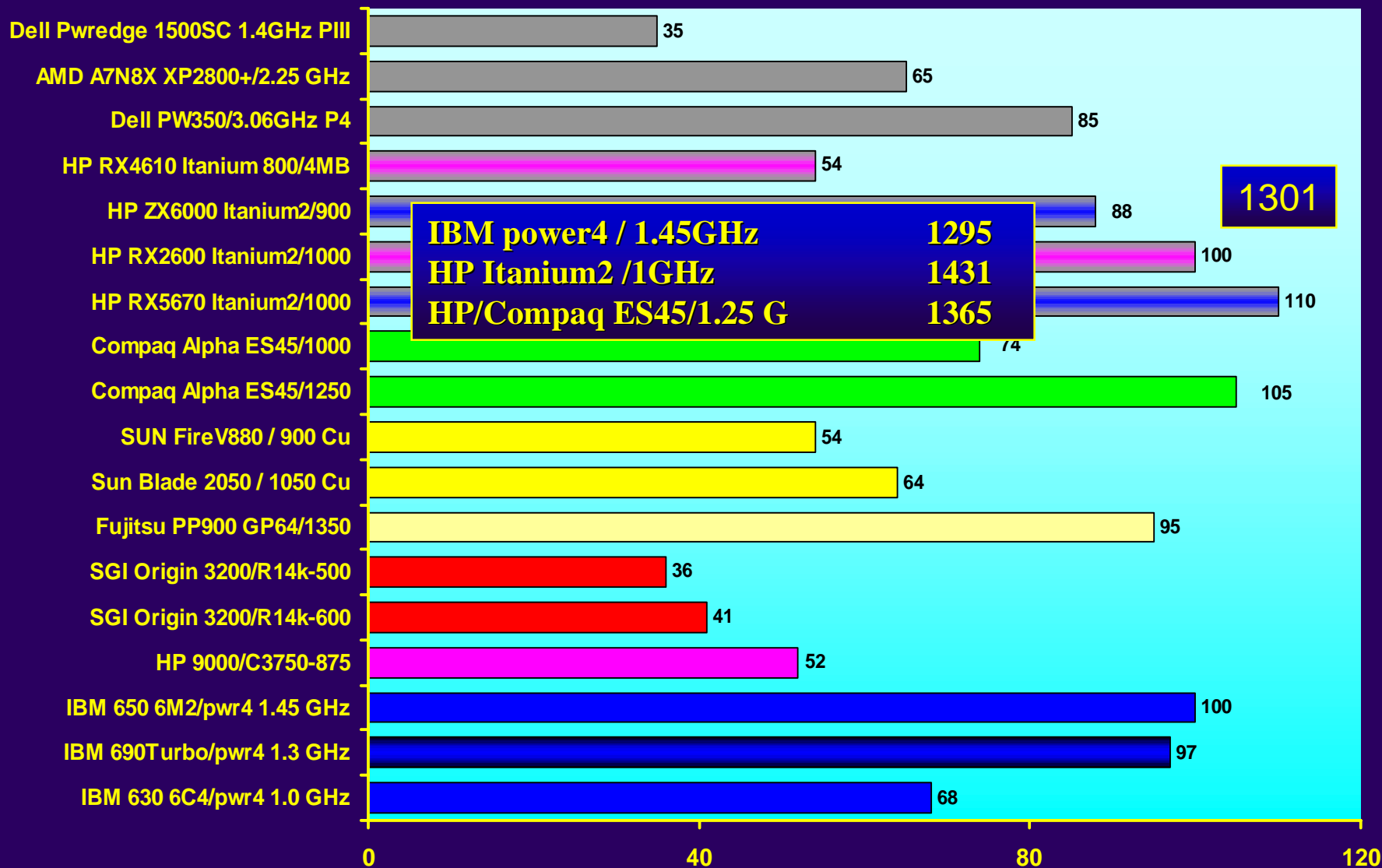
SPEC CPU 2000 - Floating point Benchmark Suite (SPECfp2000)

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.quake	C	Seismic wave propagation simulation
187.facerec	F90	Image processing: Face recognition
188.amp	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

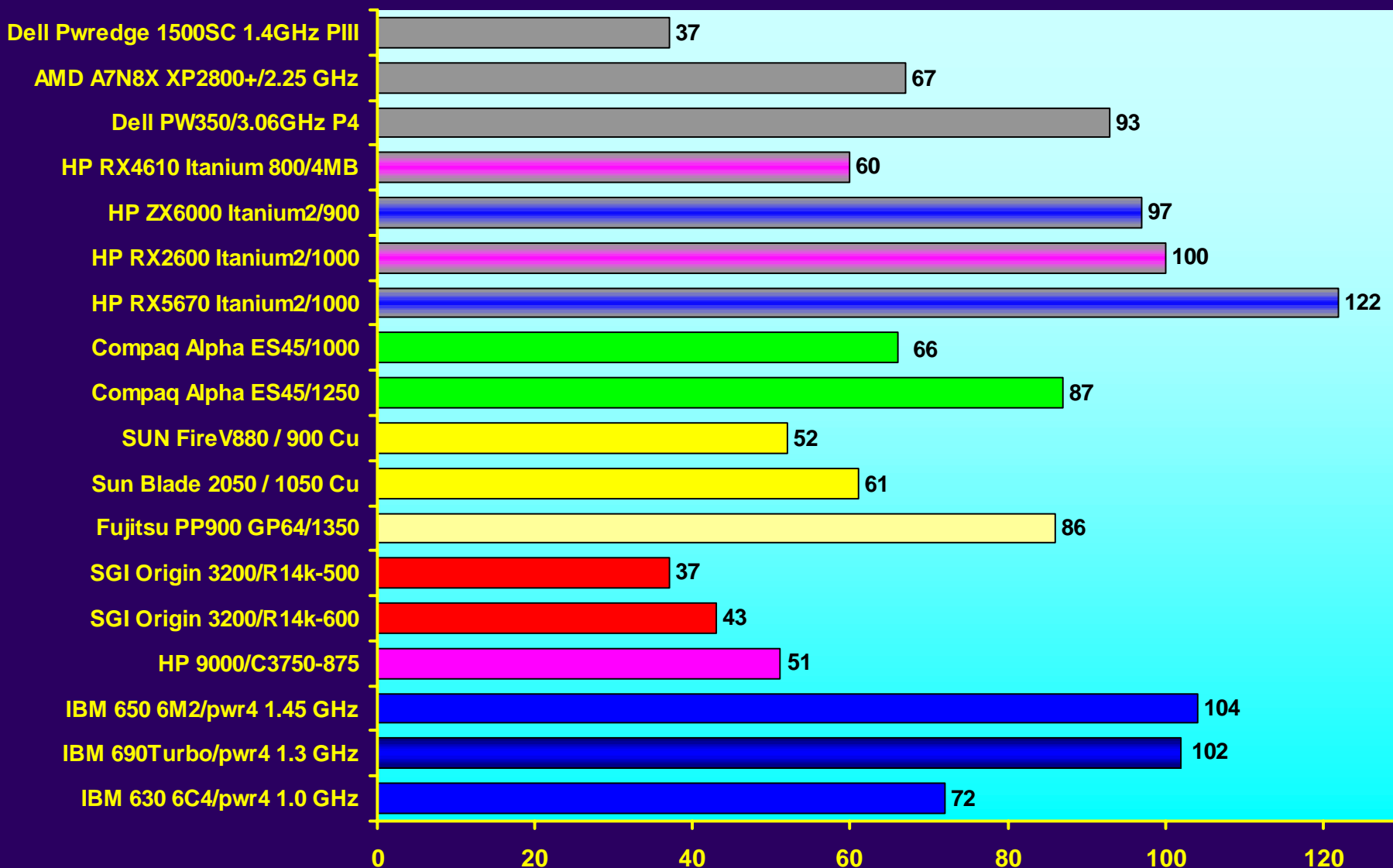
SPEC CPU 2000 - SPECfp2000

Values relative to HP RX2600 Itanium2/1000



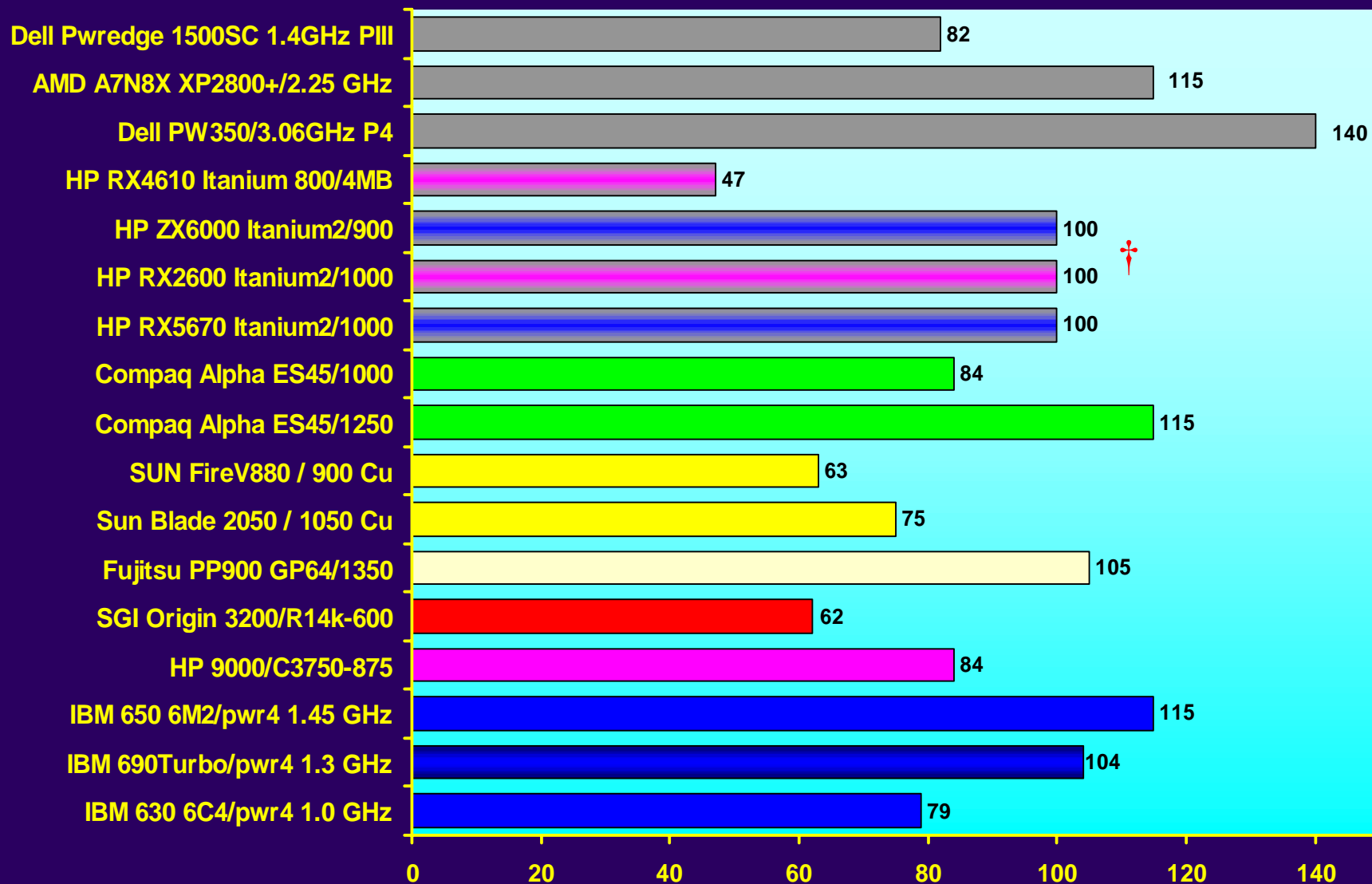
SPEC CPU 2000 - SPECfp2000_base

Values relative to HP RX2600 Itanium2/1000



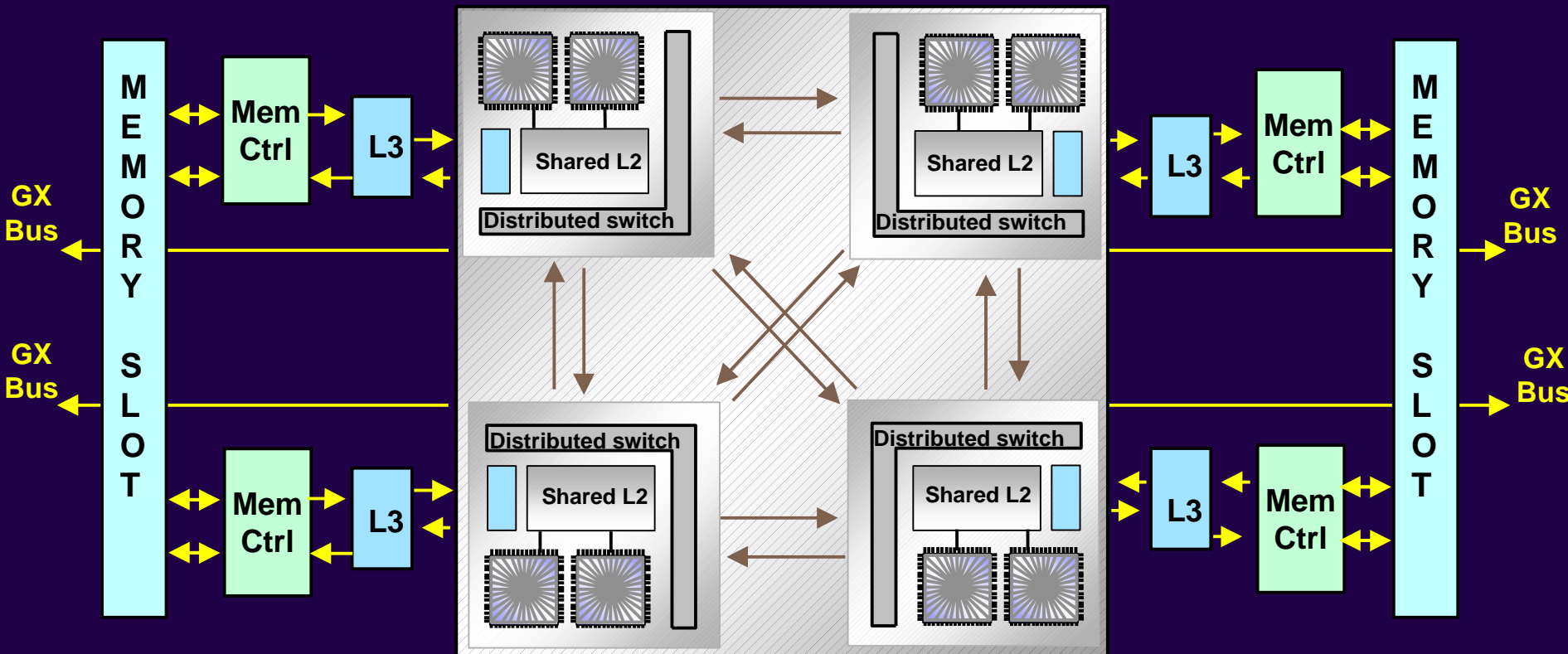
SPEC CPU 2000 - SPECint2000

Values relative to HP RX2600 Itanium2/1000



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

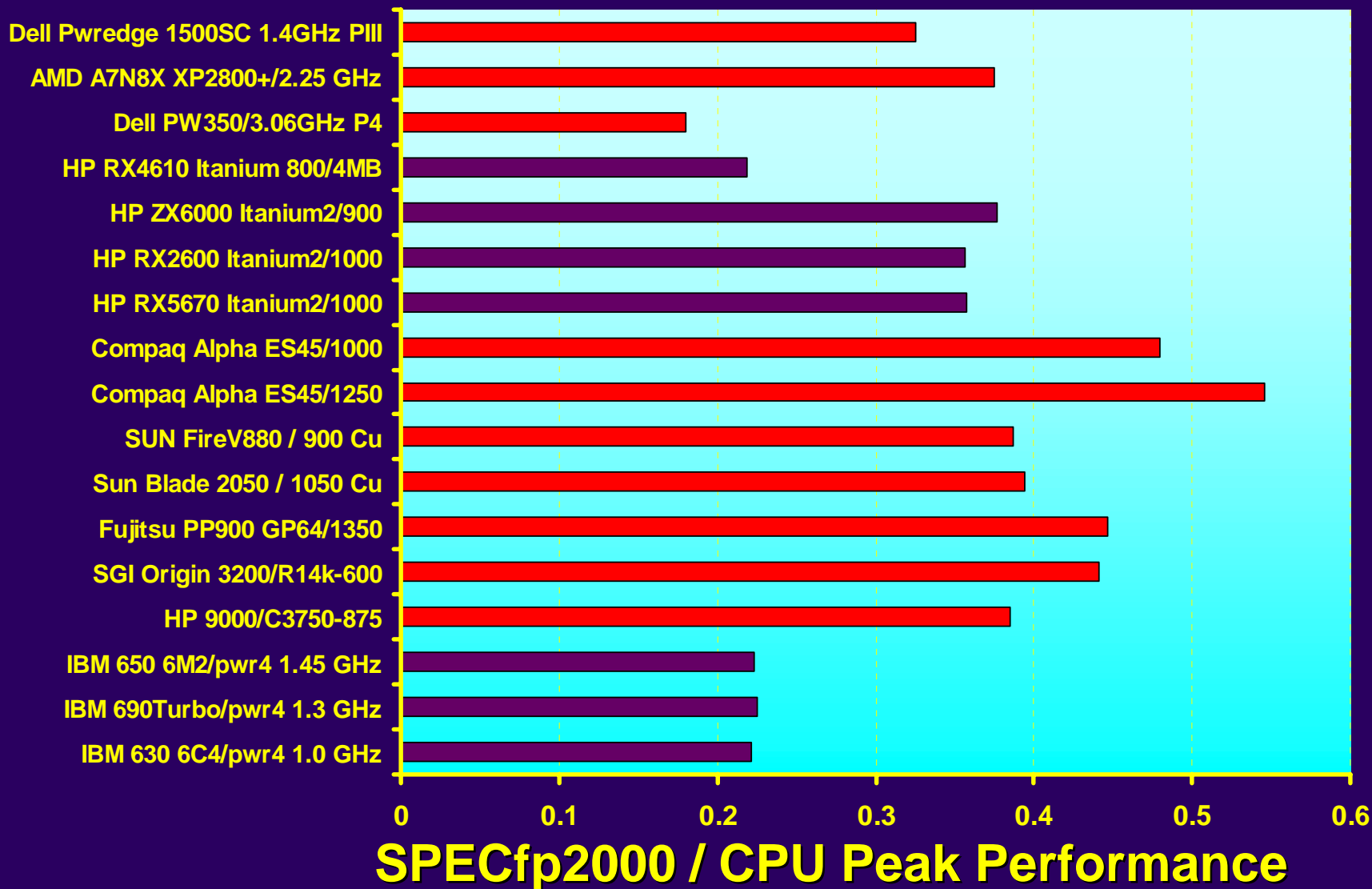
Four POWER4 chips (8 processors) on an MCM, with two associated memory slots



L3 cache shared 4 GX Bus links for external connections across all processors

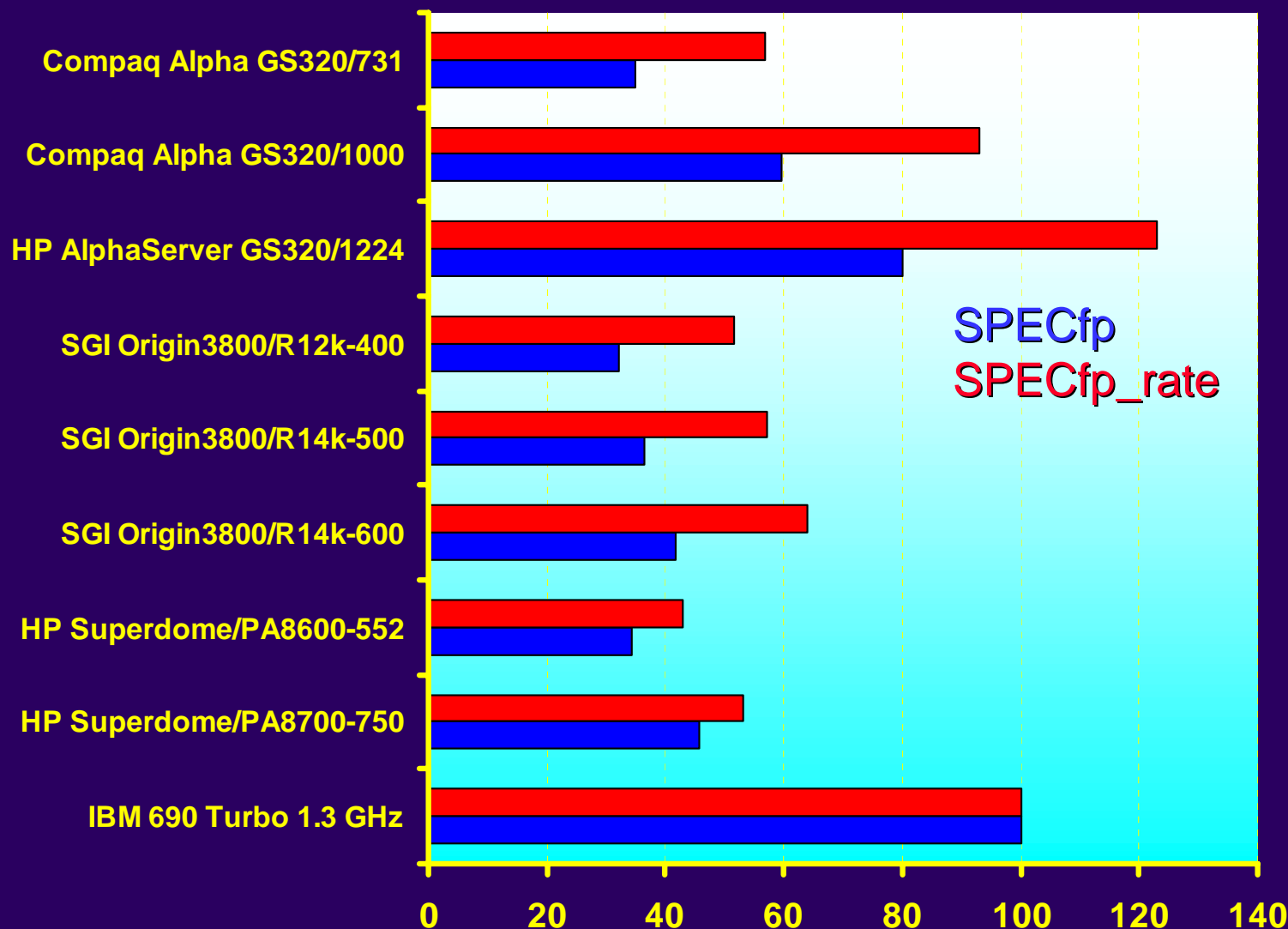
SPEC CPU 2000 - SPECfp2000

Units of SPECfp as a function of Peak Performance



SPEC CPU 2000 - SPECfp vs SPECfp_rate (32 CPUs)

Values relative to IBM 690 Turbo 1.3 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)

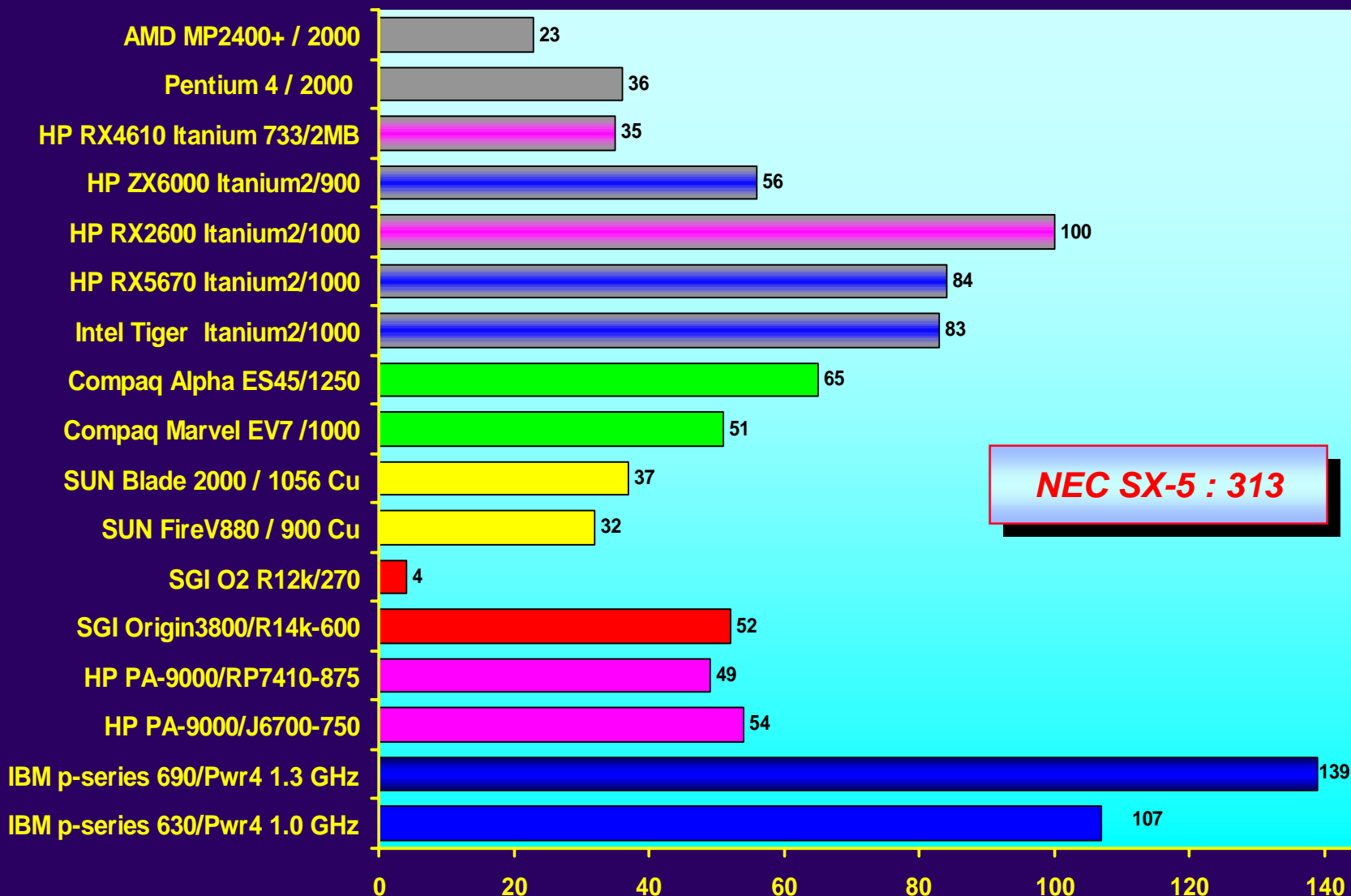
- SPARSE Matrix Multiply BenchMark
 - MMO operation is central to the efficient operation of modern QC codes. In this benchmark a series of MMOs ($R = A \times B$) are performed involving matrices of increasing order:
 - MATRIX-89: 10, 20, 30, ... , 100 (B is sparse)
 - MATRIX-97: 50, 100, 150, ... ,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

Memory bandwidth

-lblas

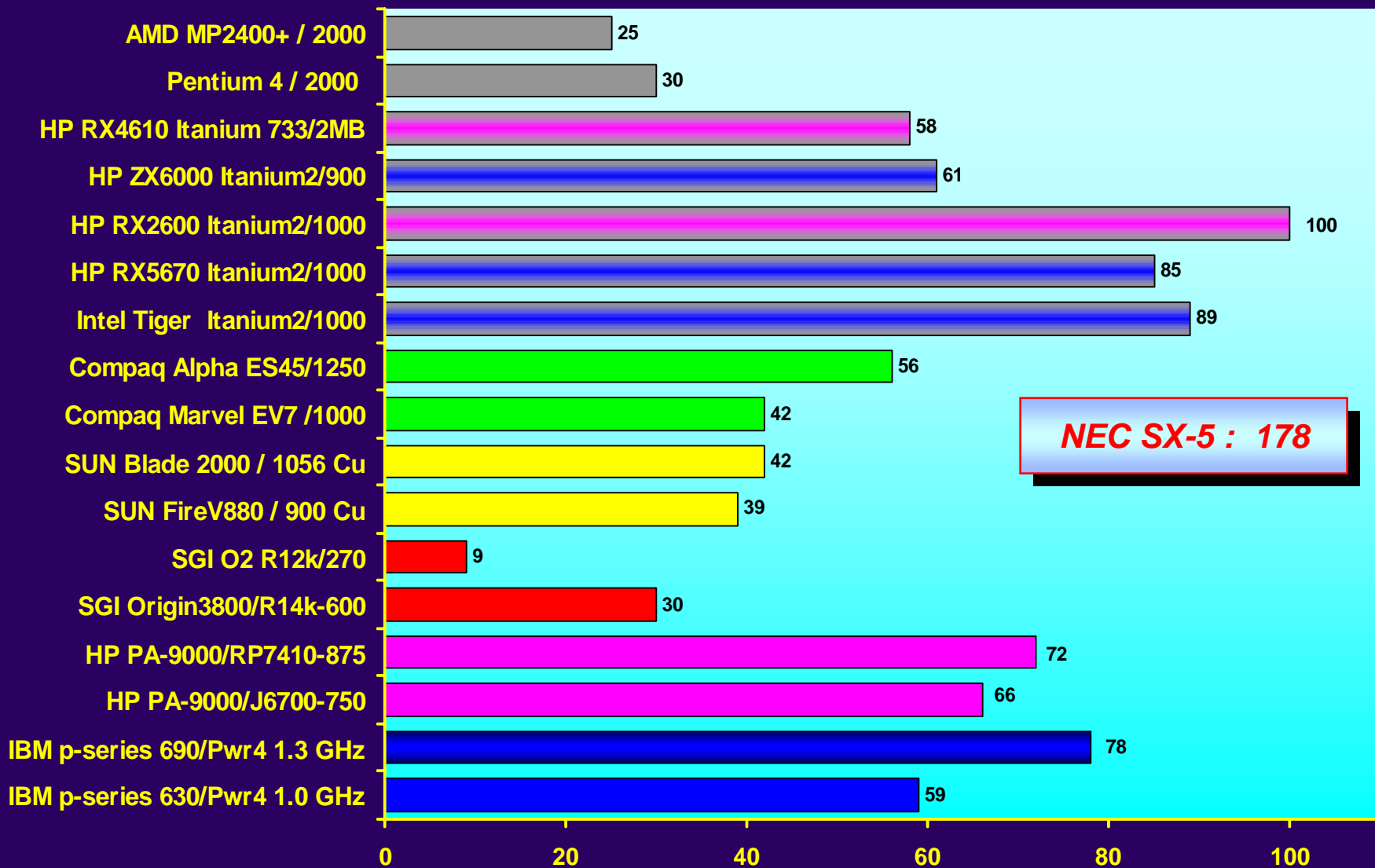
Matrix-97: SPARSE MMO Benchmark.

Performance relative to the HP RX2600 Itanium2/1000



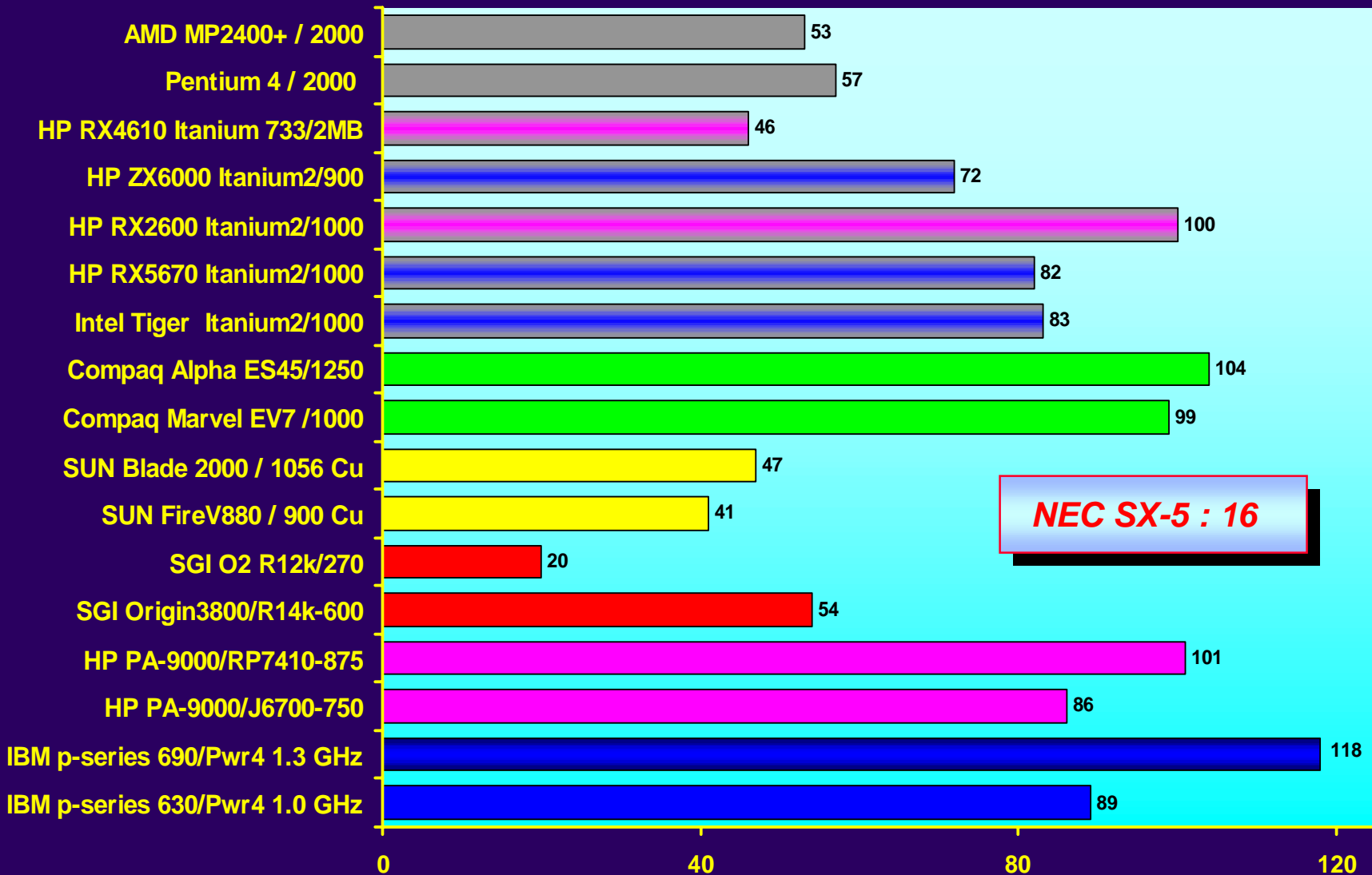
Matrix-97: Q[†]HQ MMO Benchmark.

Performance relative to the HP RX2600 Itanium2/1000



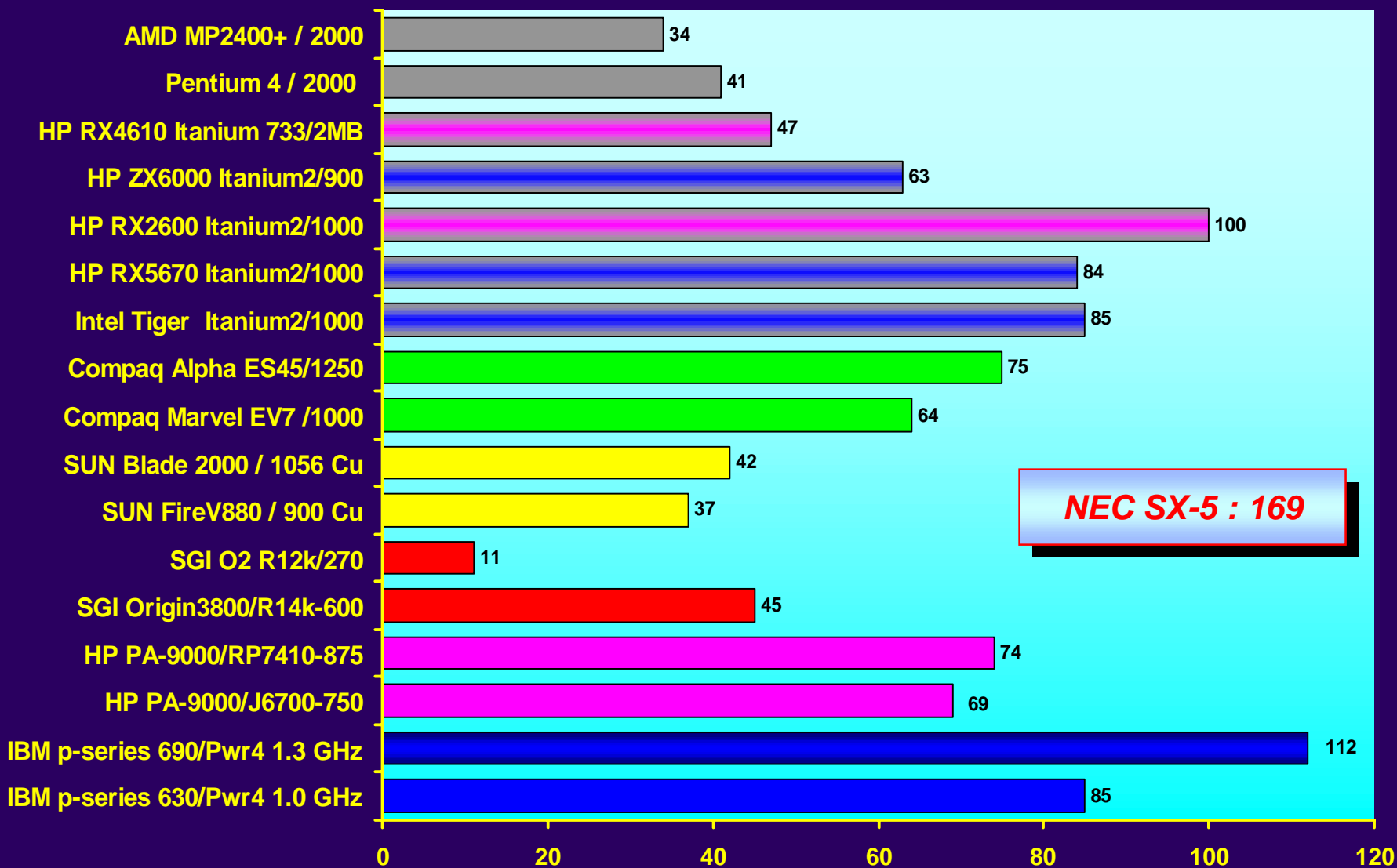
Matrix-97: Diagonalisation Benchmark

Performance relative to the HP RX2600 Itanium2/1000



The Matrix-97 Benchmarks.

Performance relative to the HP RX2600 Itanium2/1000



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 Be₄ (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)

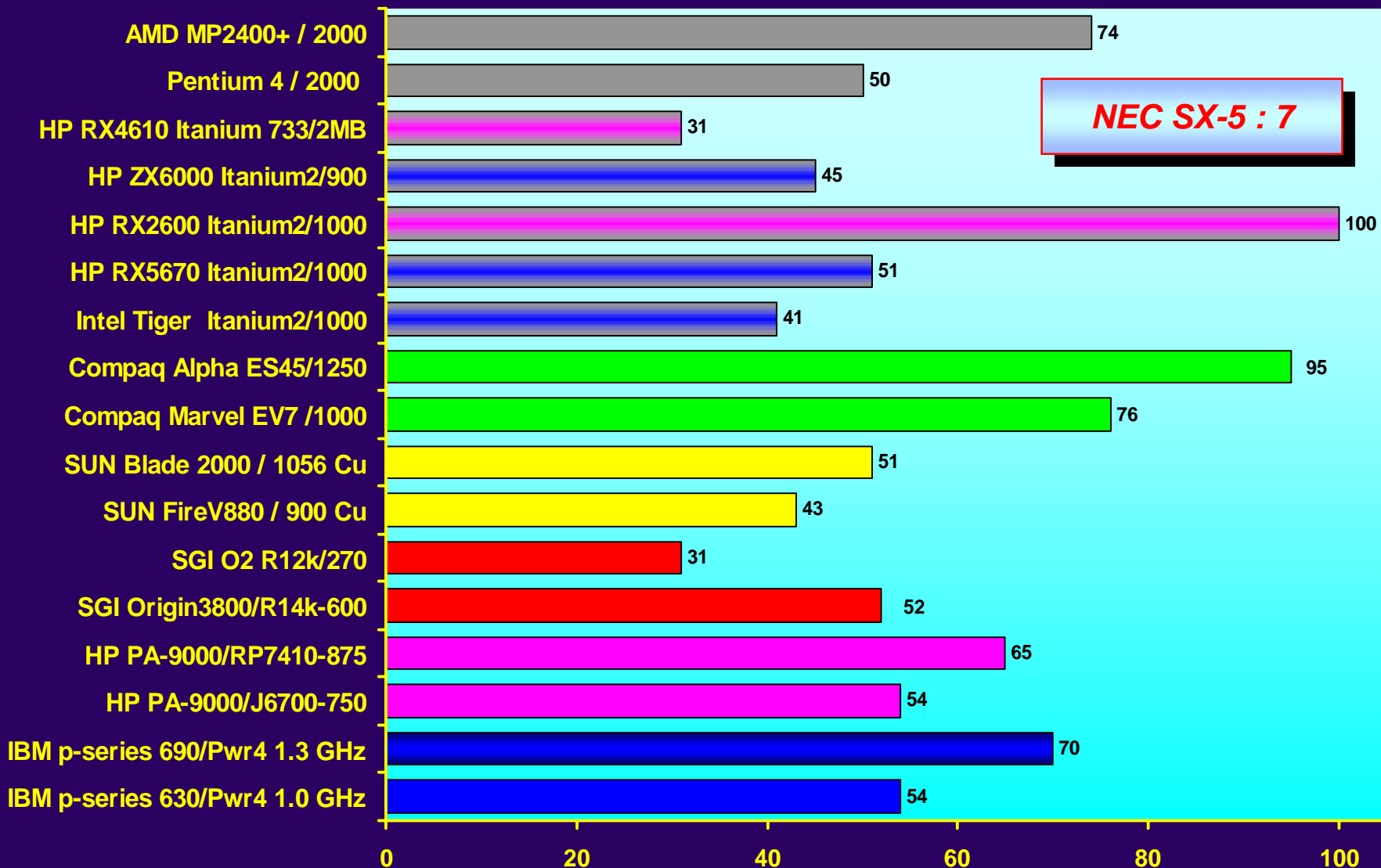
- This code evaluates the energy of the simplest explicitly correlated electronic wavefunction for the He atom using a variational monte-carlo method without importance sampling.

■ 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.

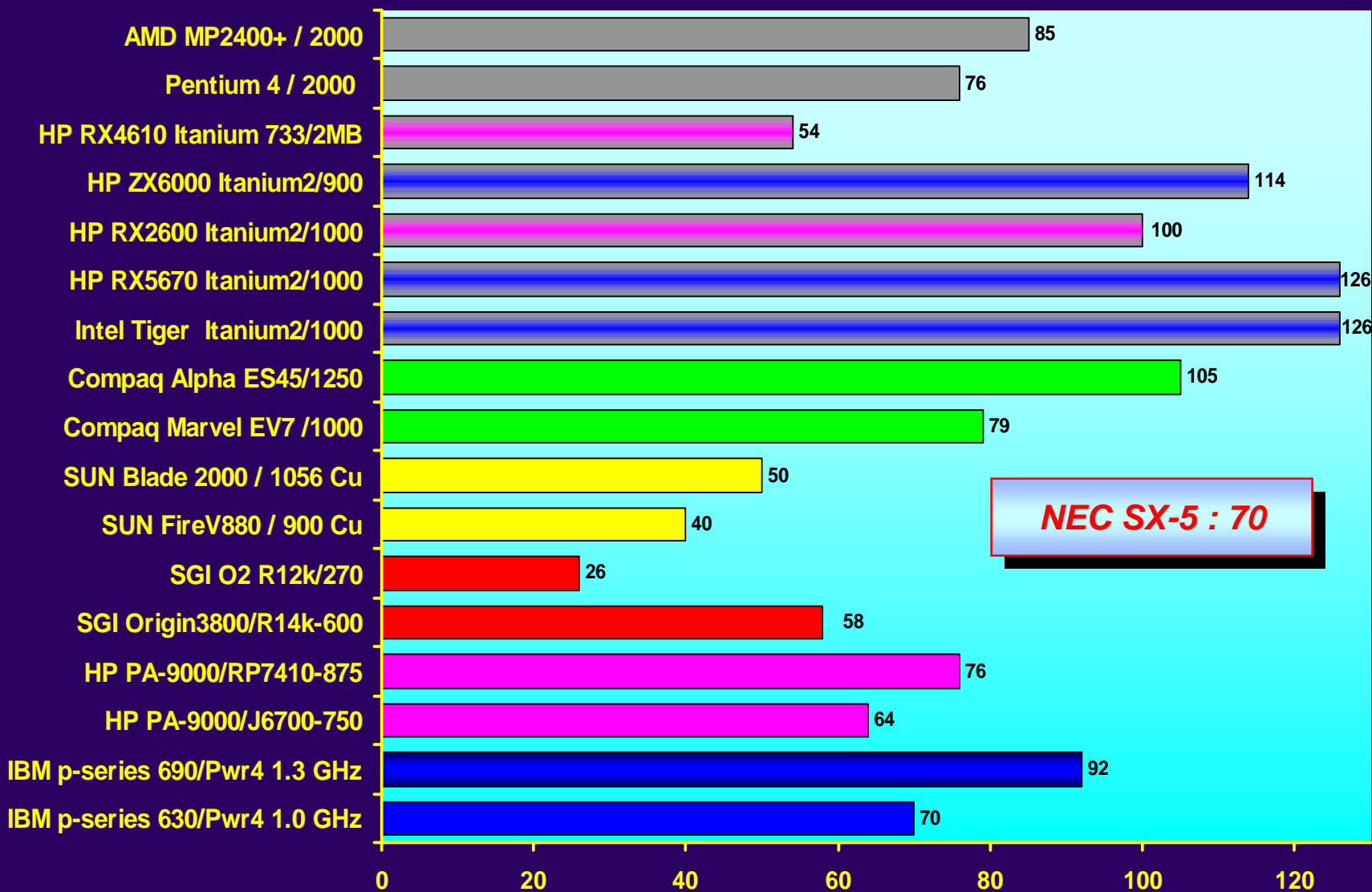
Computational Chemistry Kernels - Direct-SCF.

Performance relative to the HP RX2600 Itanium2/1000



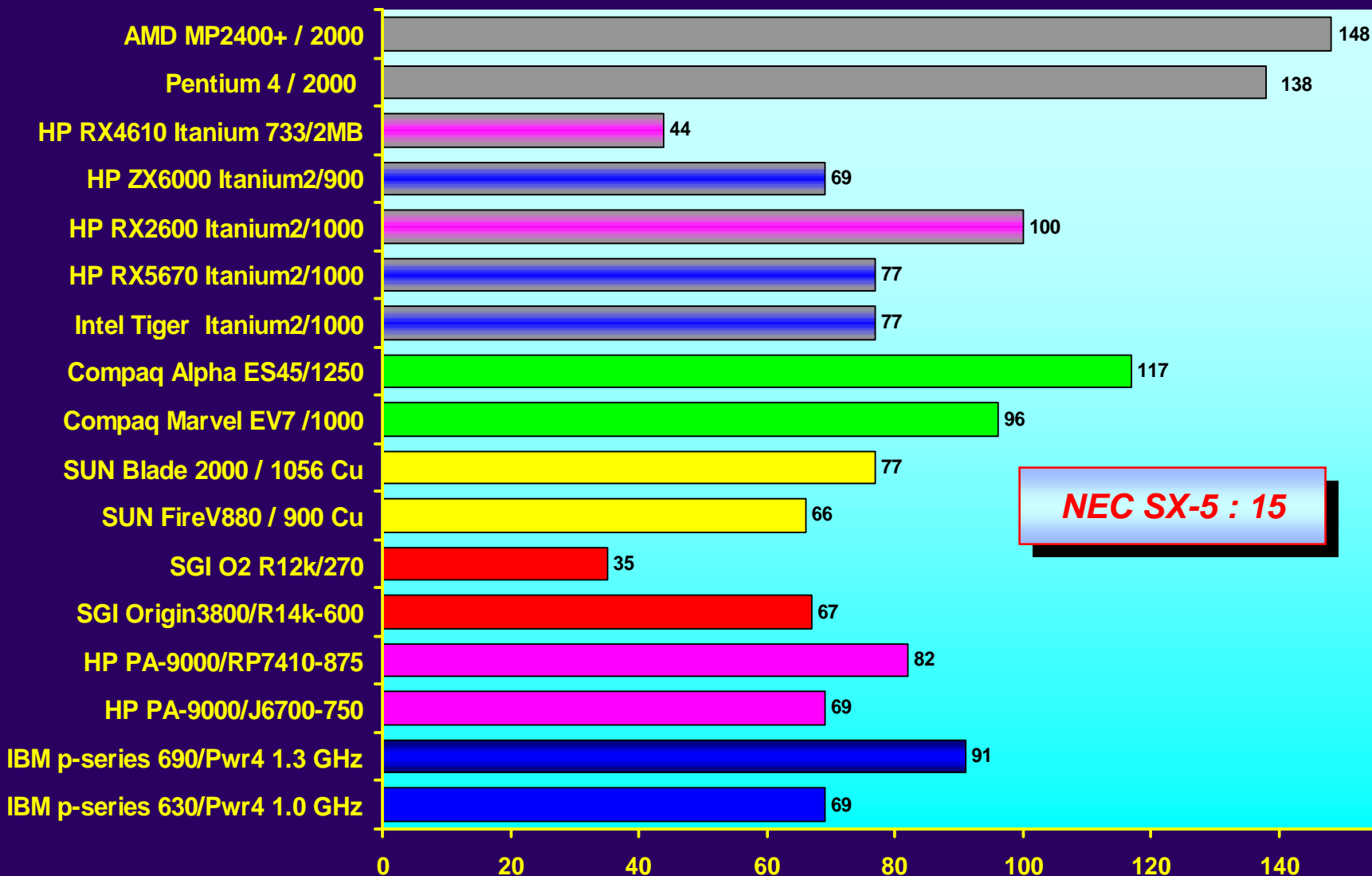
Chemistry Kernels - Molecular Dynamics.

Performance relative to the HP RX2600 Itanium2/1000



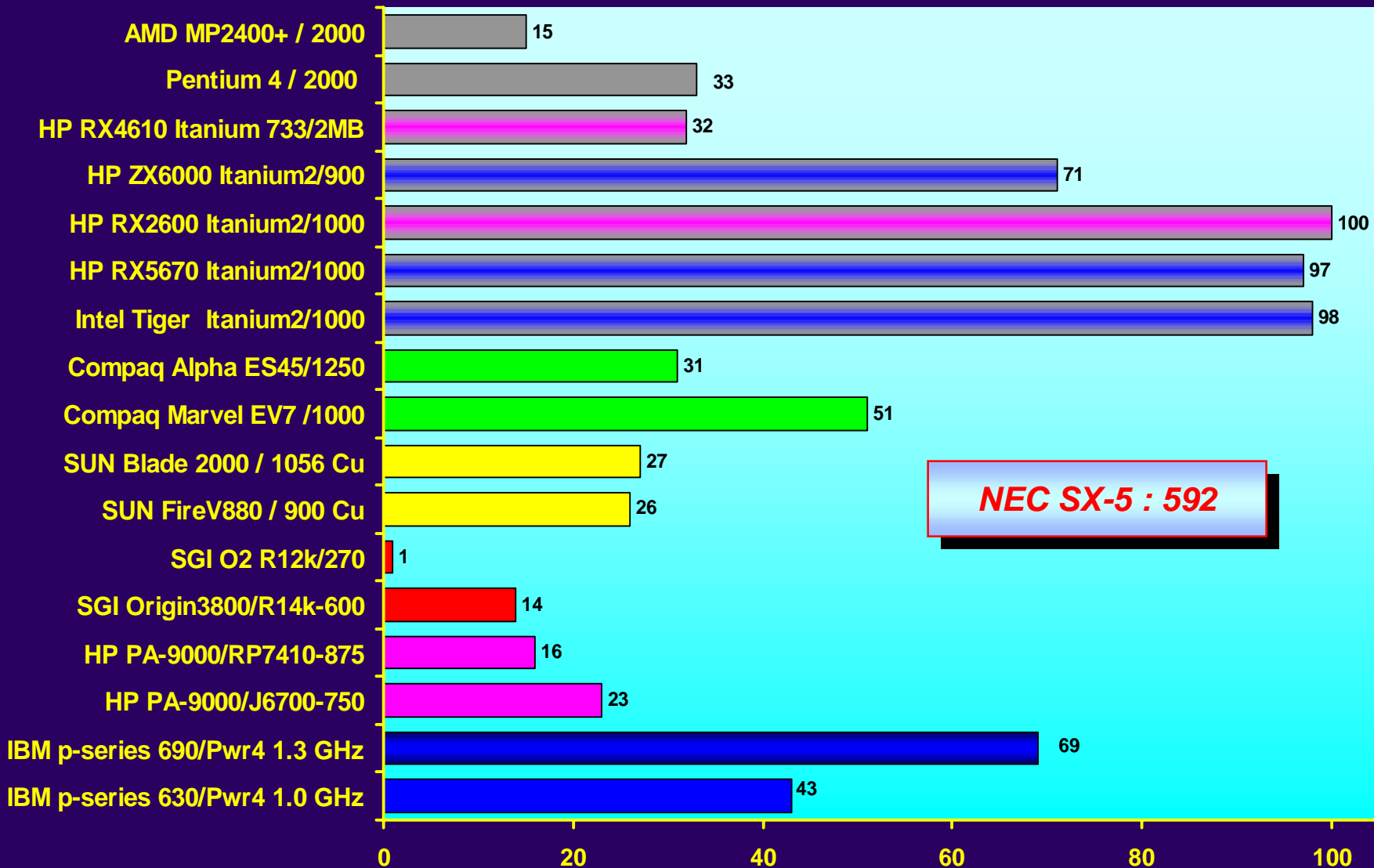
Chemistry Kernels - Quantum Monte Carlo.

Performance relative to the HP RX2600 Itanium2/1000

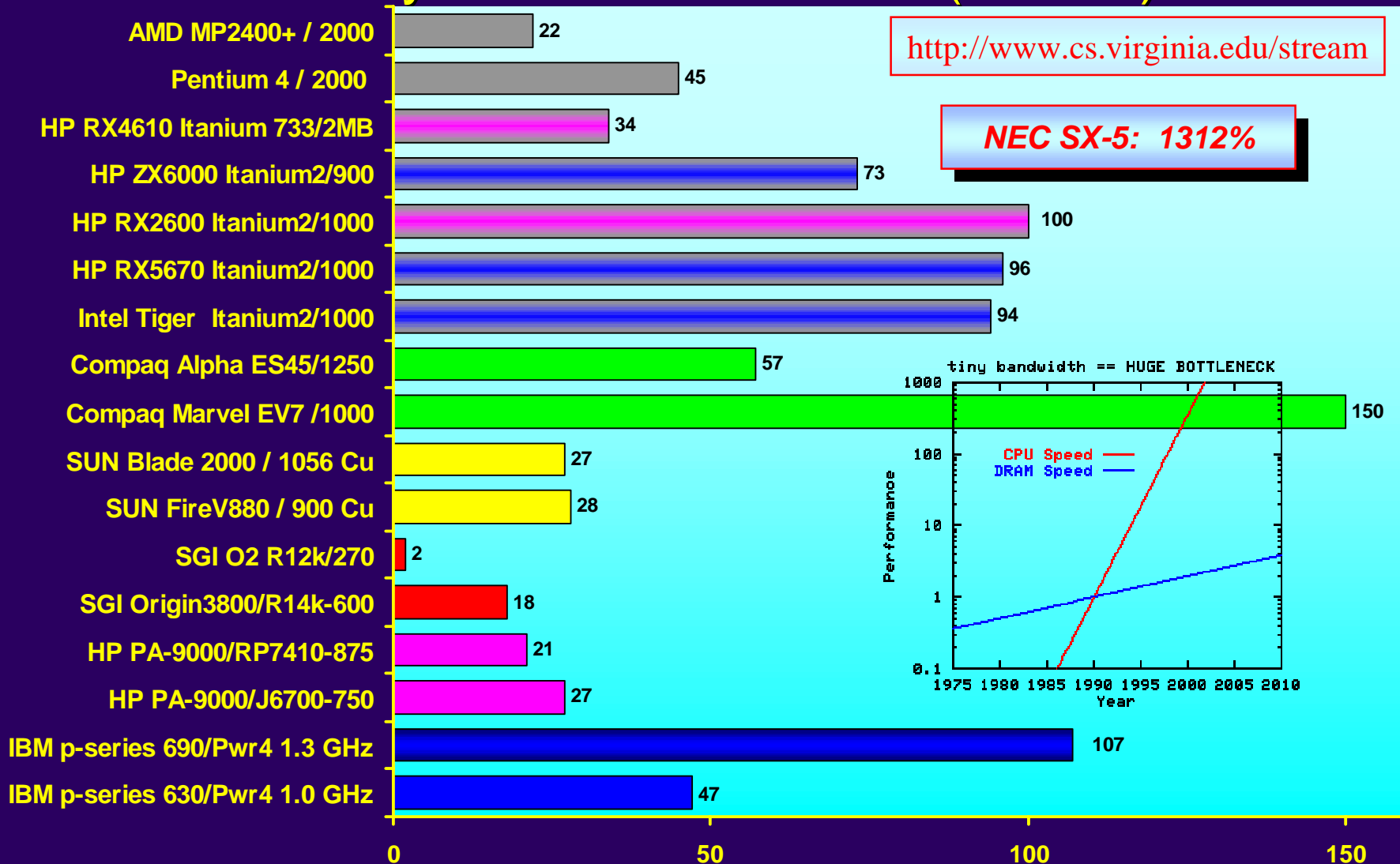


Chemistry Kernels - Jacobi Solver.

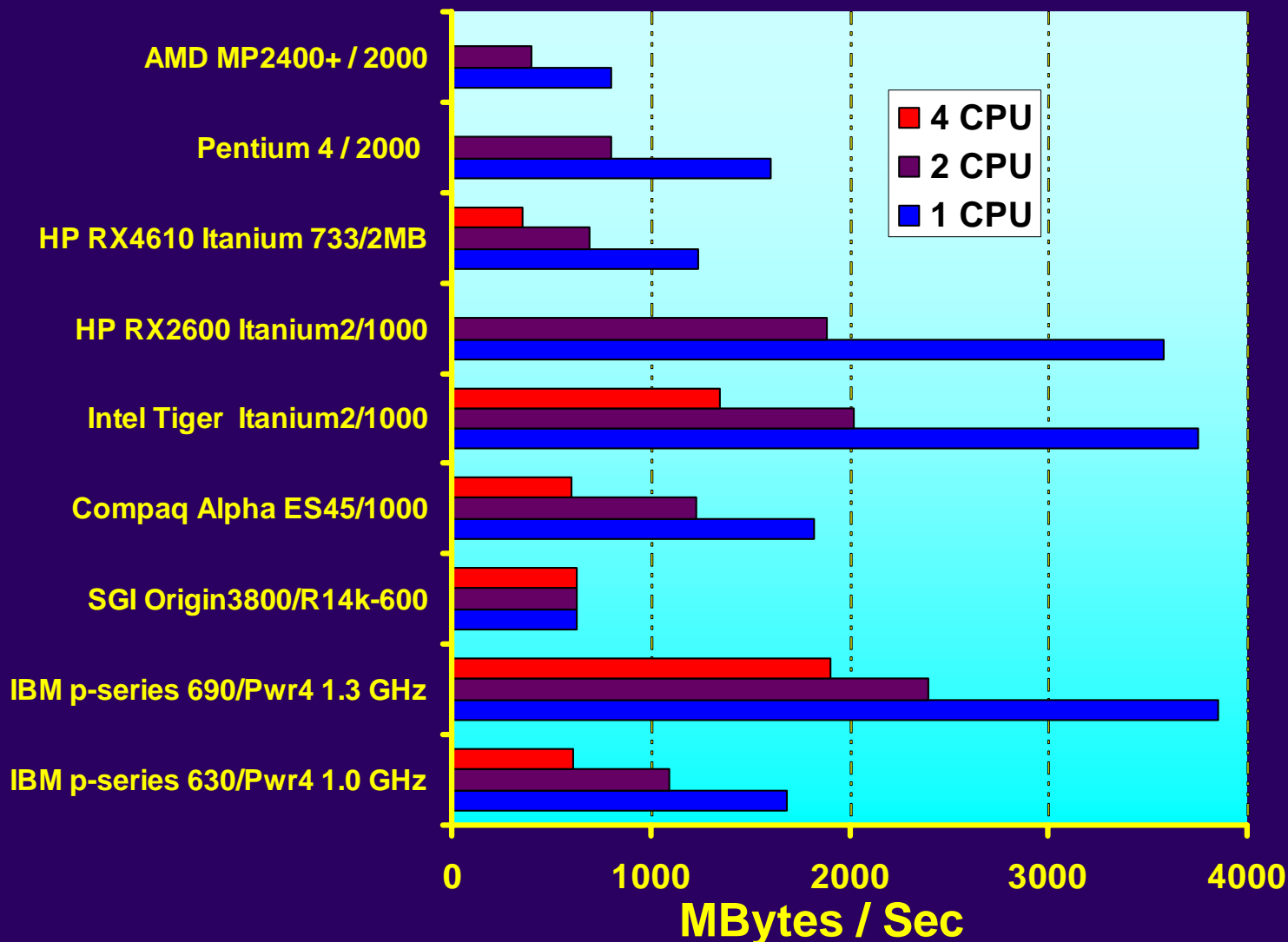
Performance relative to the HP RX2600 Itanium2/1000



STREAM: Measured Sustainable Memory Bandwidth in HPC (TRIAD)

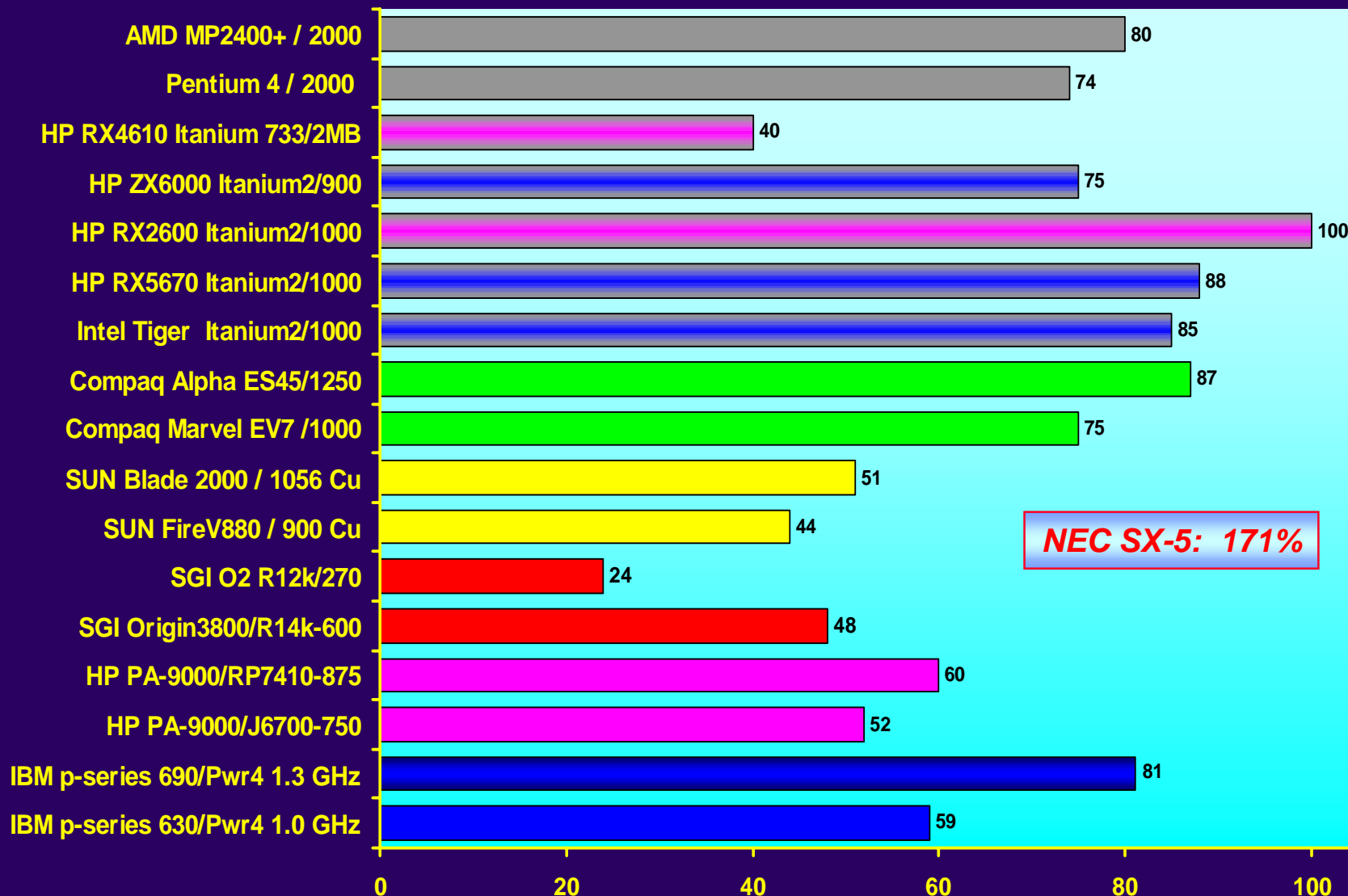


STREAM: Sustainable Memory Bandwidth (TRIAD) per process



Computational Chemistry Kernels.

Performance relative to the HP RX2600 Itanium2/1000



GAMESS-UK and DL_POLY Benchmarks

GAMESS-UK

DL_POLY

12 Typical QC Calculations

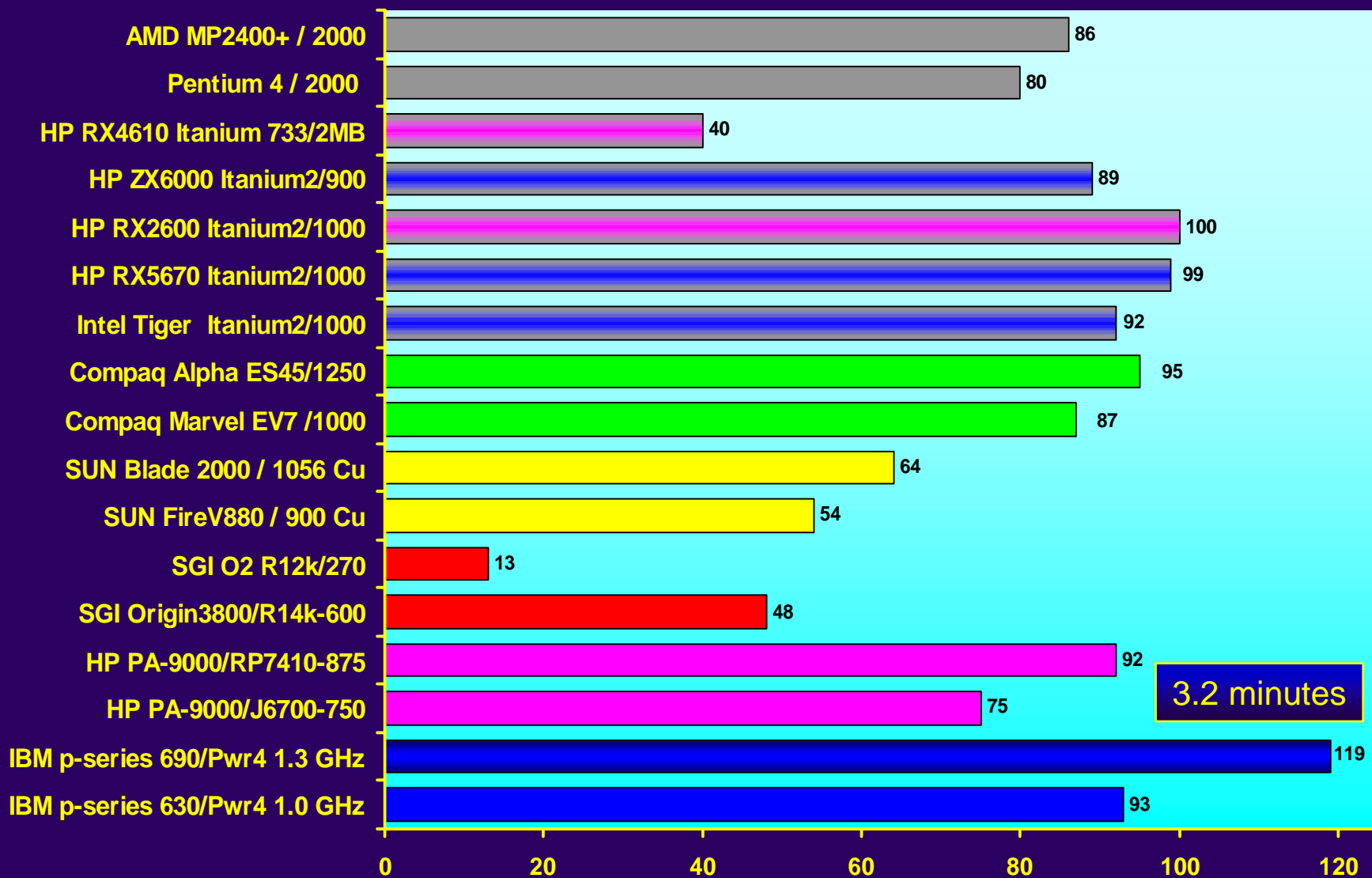
<u>Module</u>	<u>Basis (GTOs)</u>	<u>Species</u>
1. SCF	STO-3G (124)	Morphine
2. SCF	6-31G (154)	C ₆ H ₃ (NO ₂) ₃
3. ECP Geometry	ECPDZ (70)	Na ₇ Mg ⁺
4. Direct-SCF	6-31G (82)	Cytosine
5. CAS-geometry	TZVP (52)	H ₂ CO
6. MCSCF	EXT1 (74)	H ₂ CO
7. Direct-CI	EXT2 (64)	H ₂ CO/H ₂ +CO
8. MRD-CI (26M)	ECP (59)	TiCl ₄
9. MP2-geometry	6-31G* (70)	H ₃ SiNCO
10. SCF 2nd derivs.	6-31G (64)	C ₅ H ₅ N
11. MP2 2nd derivs.	6-31G* (60)	C ₄
12. Direct-MP2	DZP (76)	C ₅ H ₅ N

Six Typical Simulations

<u>Simulation</u>	<u>Atoms</u>	<u>Time steps</u>
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 MgCl ₂ 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 HP RX2600 Itanium2/1000



SPECfp2000 and the GAMESS-UK Benchmark



The GAMESS-UK-99 Benchmark

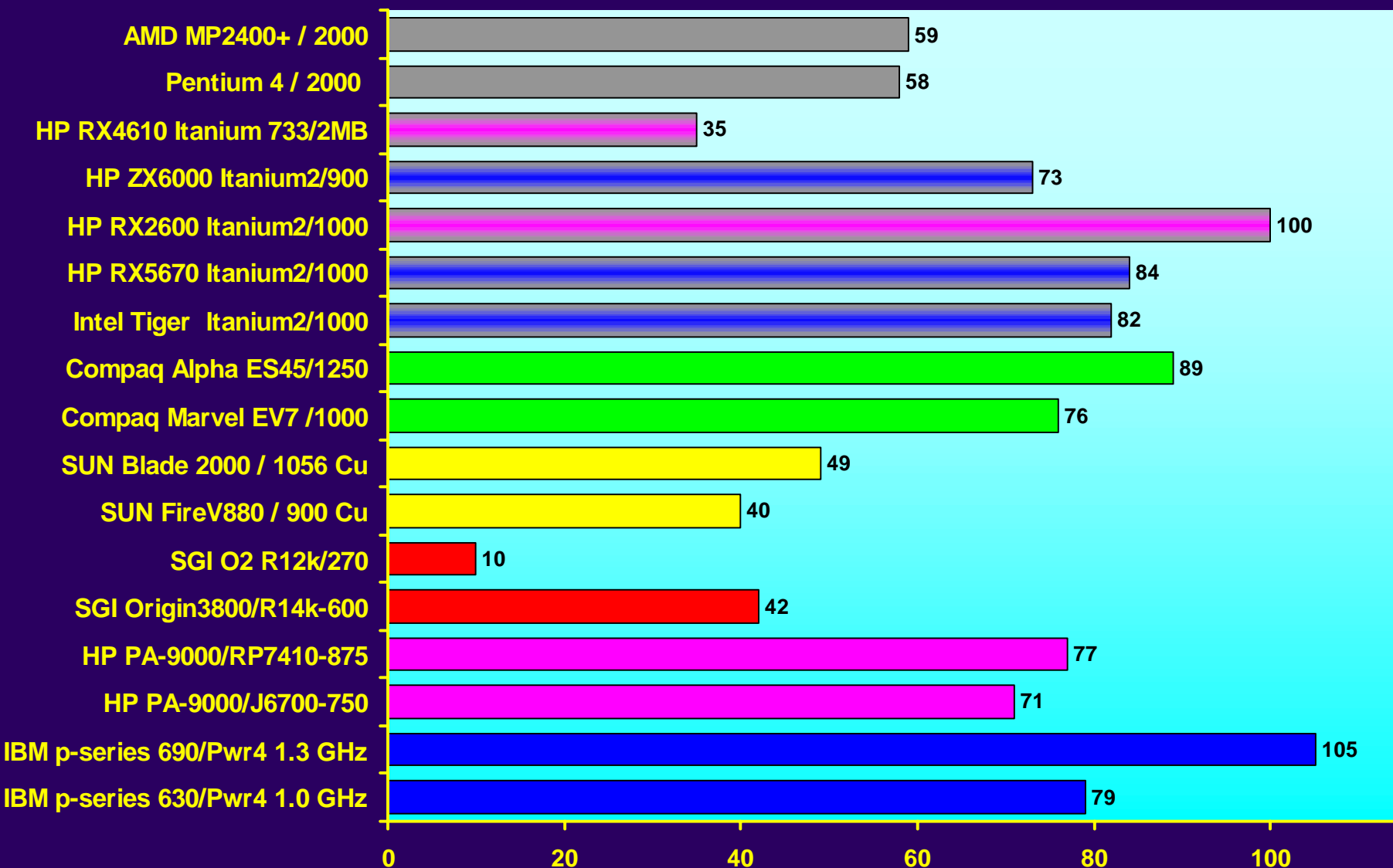
10 Typical QC Calculations

<u>Module</u>	<u>Basis (GTOs)</u>	<u>Species</u>
1. Direct- SCF	6-31G (227)	Morphine
2. SCF	6-31G** (265)	C ₆ H ₃ (NO ₂) ₃
3. DFT B3LYP	6-311G* (167)	Cytosine
4. MCSCF	CC-PVTZ (100)	H ₂ CO
5. Direct-CI	CC-PVTZ (100)	H ₂ CO/H ₂ +CO
6. CCSD(T)	TZV+2d+1f (144)	C ₄
7. MP2-geometry	TZVP (105)	H ₃ SiNCO
8. SCF 2nd derivs.	6-311G** (144)	C ₅ H ₅ N
9. MP2 2nd derivs.	TZVP(C2d) (104)	C ₄
10. Direct-MP2	6-31G* (130)	Cytosine

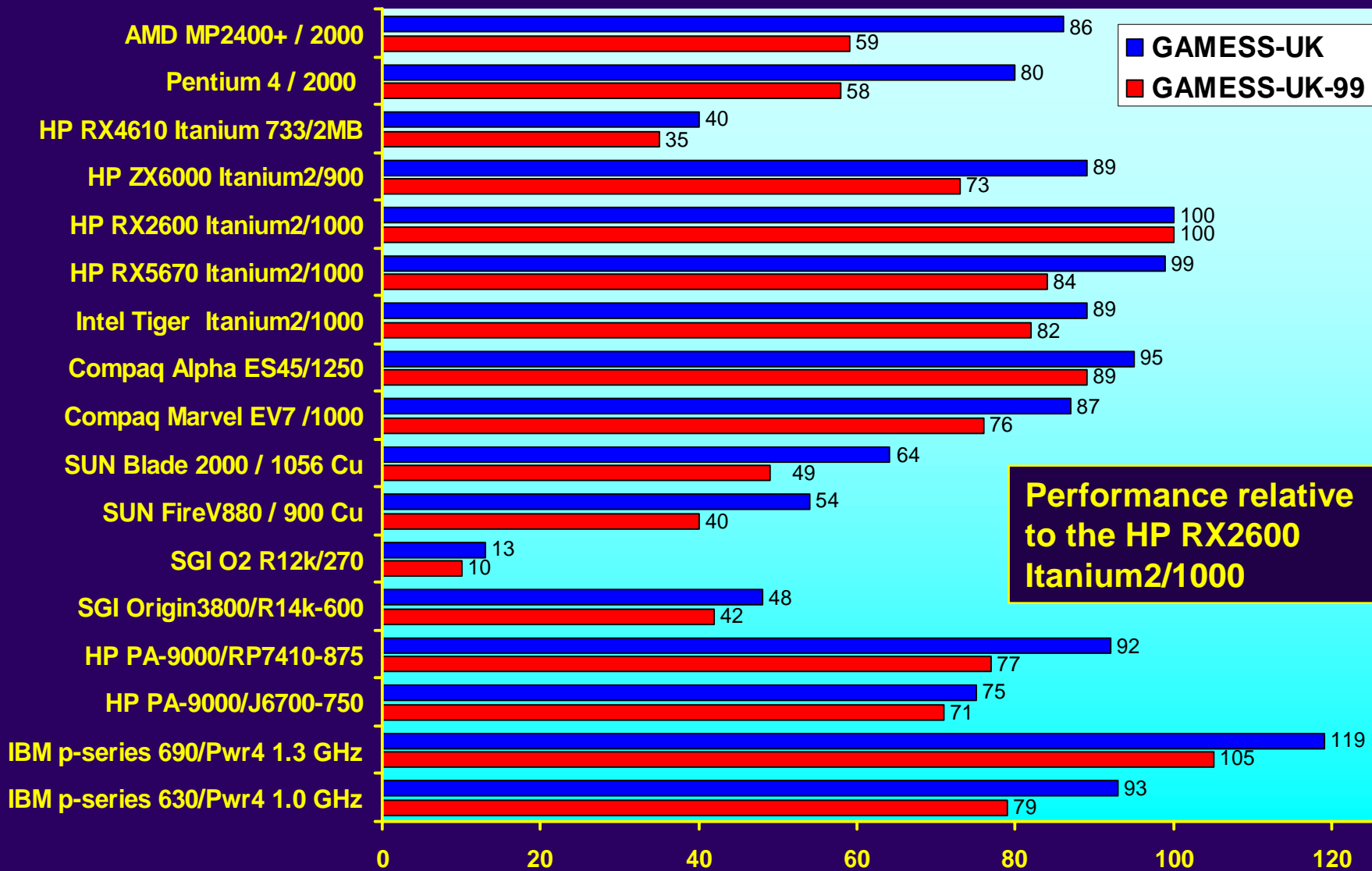
Benchmark Time: 29.8 minutes on HP RX2600 Itanium2/1000

The GAMESS-UK-99 Benchmark

Performance relative to the HP RX2600 Itanium2/1000

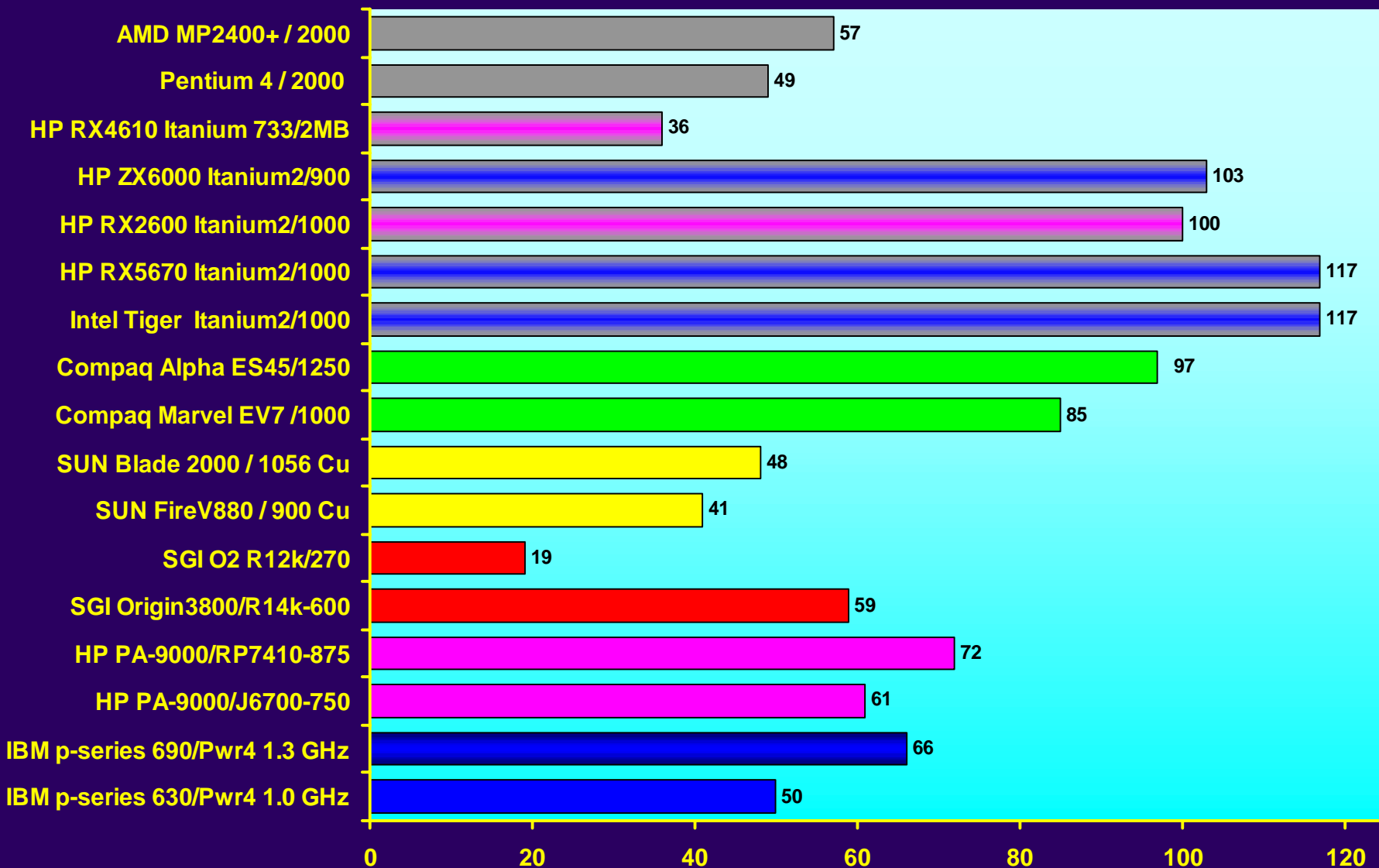


The GAMESS-UK and GAMESS-UK-99 Benchmark

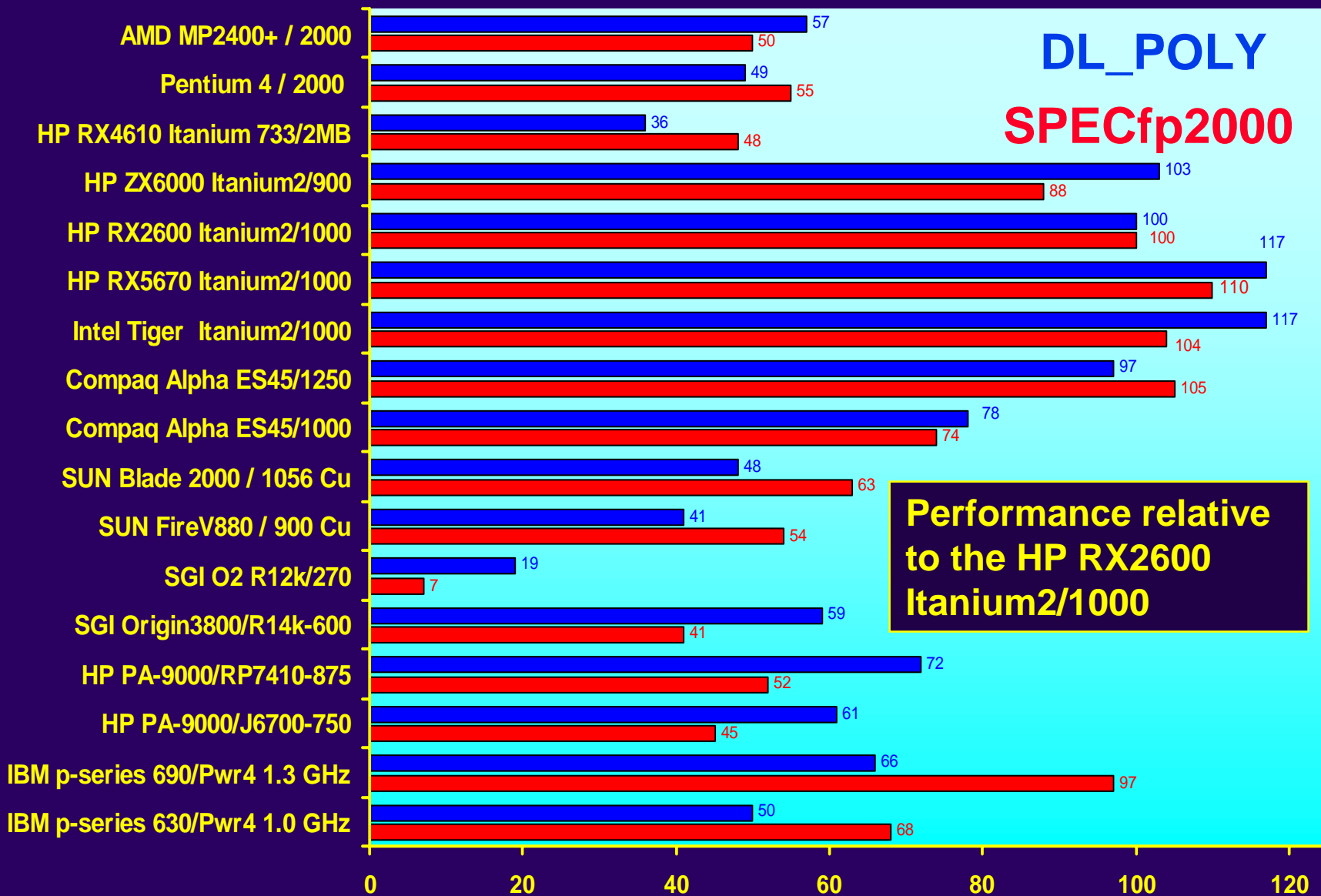


The DL_POLY Benchmark.

Performance relative to the HP RX2600 Itanium2/1000

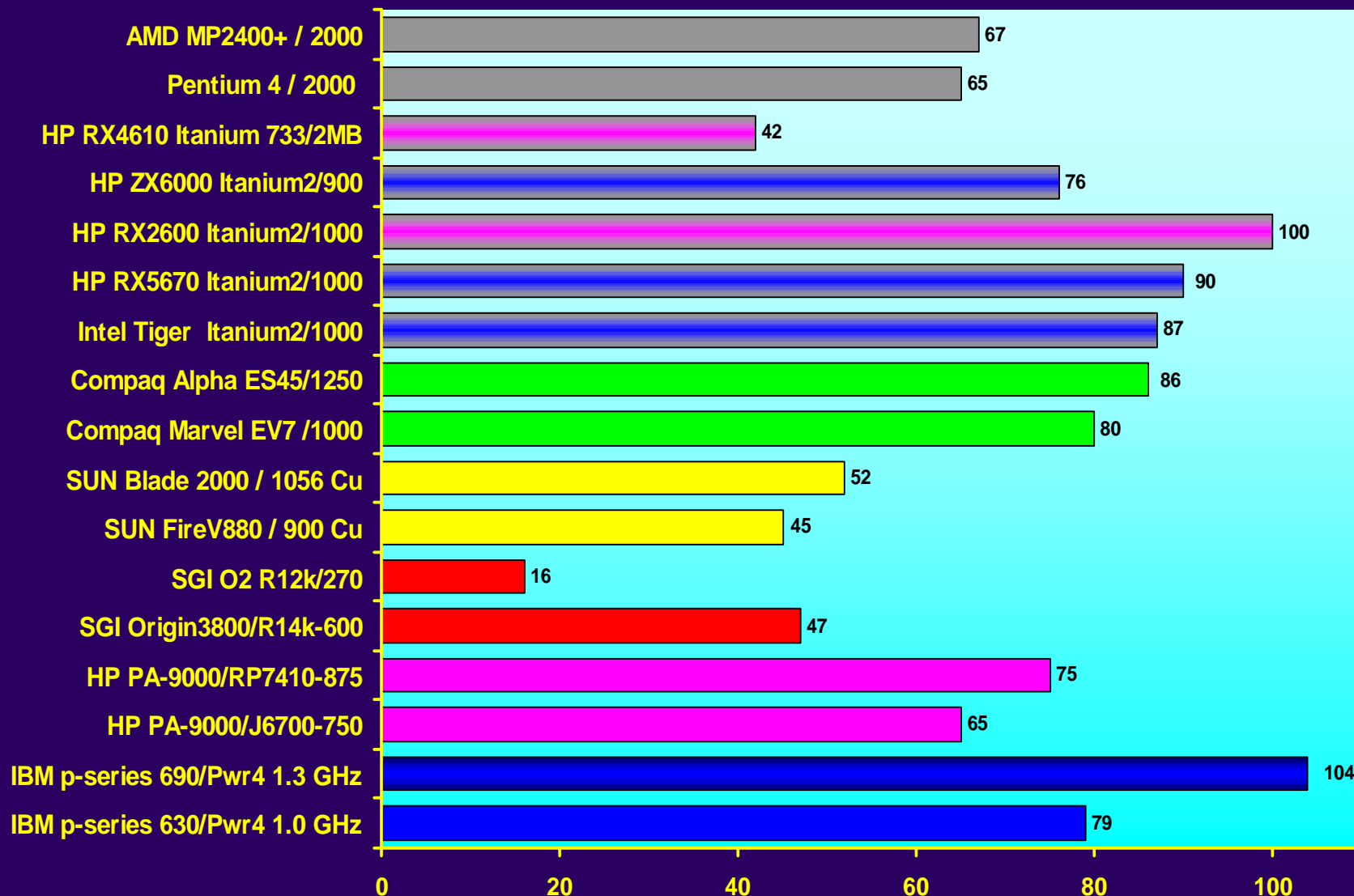


SPECfp2000 and the DL_POLY Benchmark



Summary Index relative to the HP RX2600 Itanium2/1000

The MATRIX-97, Chemistry Kernels and GAMESS-UK 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 $R_i = n \times T_{ref} / T_i$
 - T_{ref} is the elapsed time on a reference system. (*HP RX/2600 Itanium2/1000* 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 ($R = A \times B$) are performed involving matrices of increasing order:
 - MATRIX-97+: 100, 200, ... , 1200 (B is sparse)
- Diagonalisation Benchmark
 - performance of 7 routines from mathematical libraries and QC codes:
 - MATRIX-97+: 100, 200, ... , 600
- Q[†]HQ Benchmark
 - involves use of library routines e.g. BLAS. Uses both a scalar and vector algorithm (DGEMM):
 - MATRIX-97+: 100, 200, ... , 1000

Memory bandwidth

-lblas

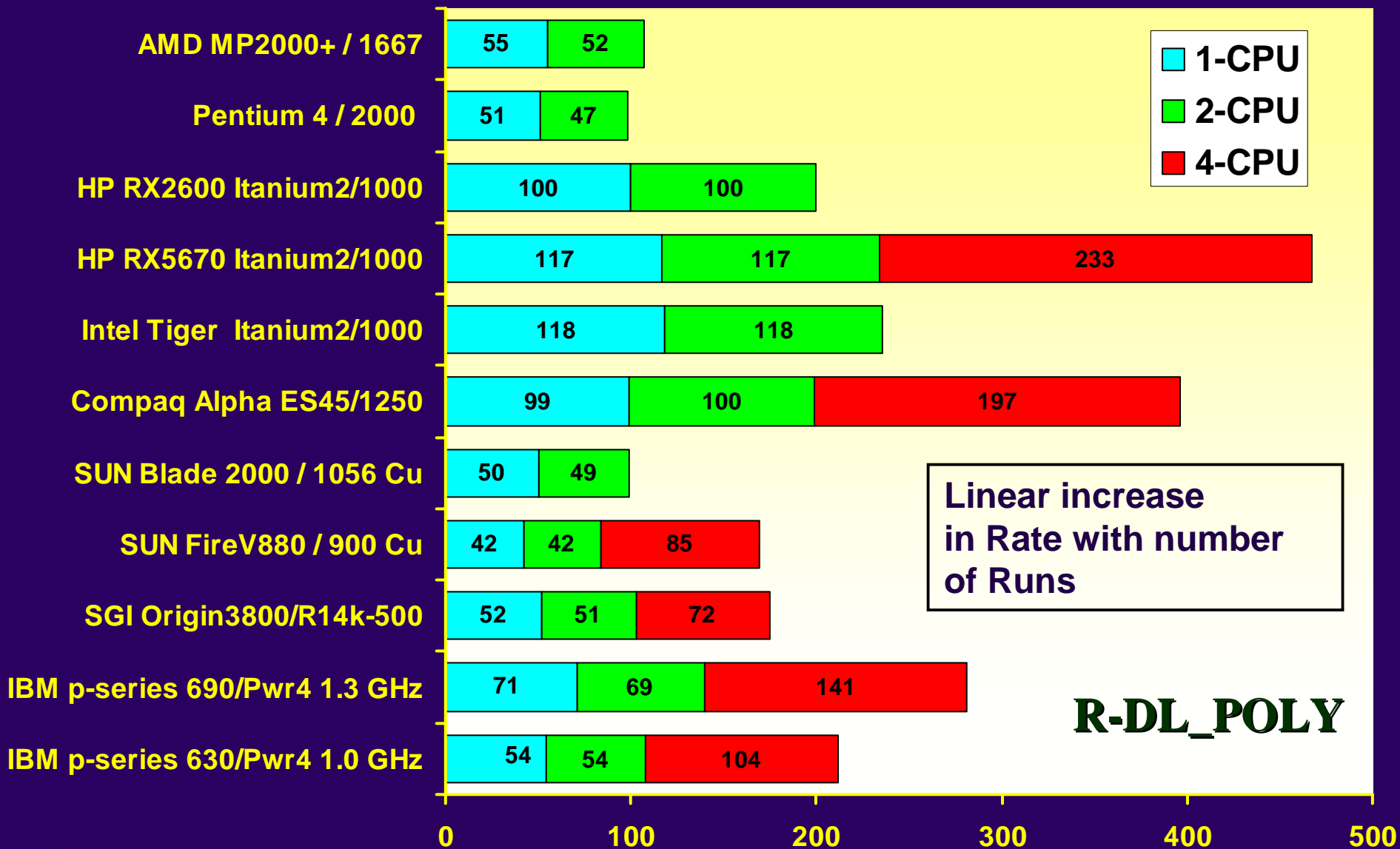
2. DLPOLY

- 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 2nd derivs., MP2 2nd derivs., Direct-MP2)

Rate Benchmark: DL_POLY Component



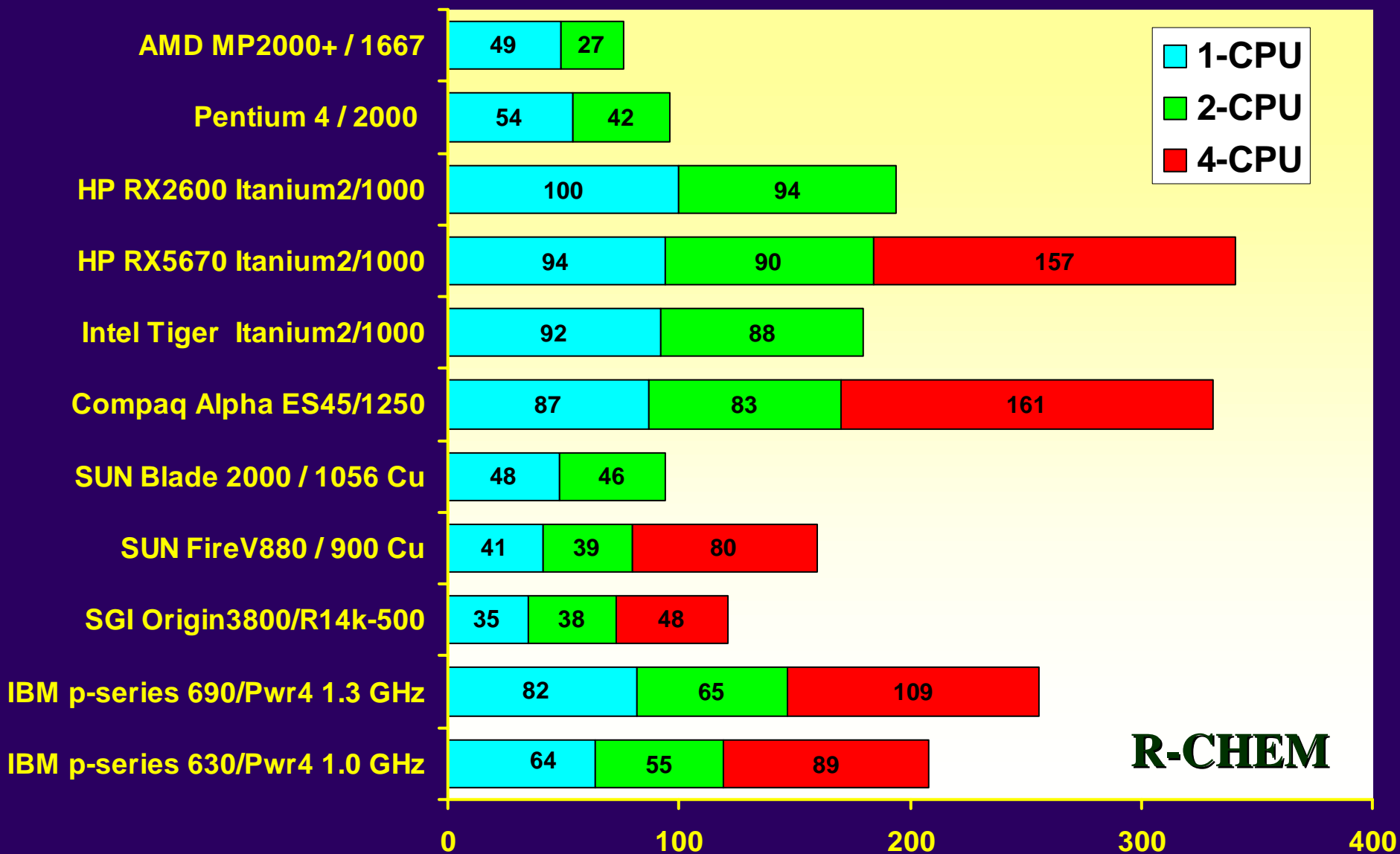
R-DL_POLY

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 $R_i = n \times T_{ref} / T_i$
 - T_{ref} is the elapsed time on the HP RX2600 / Itanium 2 scaled to a single CPU time of 100 units.

$$R_{CHEM} = 0.1 \times R_{DGEMM} + \\ 0.1 \times R_{Diagonalisation} + \\ 0.4 \times R_{DLPOLY} + \\ 0.4 \times R_{GAMESS-UK}$$

Chemistry Rate Benchmark



R-CHEM

SUMMARY

- Processor Performance Overview
 - Single-processor performance, Performance Metrics
- SPECfp and Computational Chemistry Benchmark (serial)
 - Comparison involves 200+ computers (supercomputers, workstations, PCs and MPP nodes)
 - 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>