PC workstations in crystallography

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With the advent of the Intel Pentium CPU a new class of workstations for scientific use have become available. They differ from other workstations mainly in one point: they are 5 to 10 times cheaper, while offering equal or higher performance. The price-performance advantage of these *personal* workstations is a result of the mass-market nature of PCs, as opposed to the low volume sales of would-be *real* workstations. With 90MHz Pentium CPUs they are about as fast as IBM RS/6000-550 or Silicon Graphics Indigo2 and 1.2 to 1.5 times faster than SUN Sparc 10/50. A typical, real life comparison – based on manufacturer's offers and market prices – might look like the following example:

- SGI Indigo 2 with 128 MB memory/2 GB disk – 11,600,000 Yen
- Pentium WS with 128 MB memory/10 GB disk – 1,600,000 Yen

Both machines in this comparison have roughly equal performance. An illustration of the performance using the refinement program PROLSQ is shown in the table below. The last line shows the possibility for parallel computing using co-processor boards.

System or CPU	Time	Ratio	System or CPU	Time	Ratio
VAX 11/780	1420.7	1.0	i860-50MHz	36.0	39.5
80486DX-50MHz	151.2	9.4	IBM RS/6000-550	28.4	50.0
VaxStation 4000/60	145.6	9.8	IBM RS/6000-580	18.4	77.2
SGI Crimson	37.3	38.1	Fujitsu VP-50	13.2	107.6
Pentium-90MHz	36.6	38.8	IBM RS/6000-590	12.0	118.4
i860-25MHz	53.6	26.5	4xi860-25MHz	19.8	71.6

Pentium-based workstations can be run using **linux**, a free UNIX implementation. All the source code for **linux** is available and the available software is more complete than standard commercial UNIX implementations.

We have successfully ported a variety of crystallographic programs to be used on Pentium workstations running **linux**. These include:

powder diffraction	RIETAN
small molecules	MULTAN 80 and 87, SHELXS-86, SHELXL93, ORTEP
protein structures	PROLSQ, FRODO, XTALVIEW, PROTEIN, CCP4, XPLOR

Porting is easiest for programs, which use standard language features of C or Fortran77. Programs, which use vendor-specific features, particularly DEC Fortran extensions, require more efforts. A particularly difficult example was W. Steigemann's PROTEIN system, as the VAX/VMS version was used as a starting point. Our Pentium workstations are networked using TCP/IP for communication and NFS for file sharing. Graphics is implemented through the X11 window system.