Recent Advances in PC-Linux Systems for Electronic Structure Computations by Optimized Compilers and Numerical Libraries

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One of the most frequently used packages for electronic structure research, GAUSSIAN 98, is compiled on Linux systems with various hardware configurations, including AMD Athlon (with the "Thunderbird" core), AthlonMP, and AthlonXP (with the "Palomino" core) systems as well as the Intel Pentium 4 (with the "Willamette" core) machines. The default PGI FORTRAN compiler (**pgf77**) and the Intel FORTRAN compiler (**ifc**) are respectively employed with different architectural optimization options to compile GAUSSIAN 98 and test the performance improvement. In addition to the BLAS library included in revision A.11 of this package, the Automatically Tuned Linear Algebra Software (ATLAS) library is linked against the binary executables to improve the performance. Various Hartree−Fock, density-functional theories, and the MP2 calculations are done for benchmarking purposes. It is found that the combination of **ifc** with ATLAS library gives the best performance for GAUSSIAN 98 on all of these PC-Linux computers, including AMD and Intel CPUs. Even on AMD systems, the Intel FORTRAN compiler invariably produces binaries with better performance than **pgf77**. The enhancement provided by the ATLAS library is more significant for post-Hartree−Fock calculations. The performance on one single CPU is potentially as good as that on an Alpha 21264A workstation or an SGI supercomputer. The floating-point marks by SpecFP2000 have similar trends to the results of GAUSSIAN 98 package.

INTRODUCTION

Computational chemists have been searching for computers with higher processor speed and lower price to do the calculations. Ever since the performance of personal computers (PCs) begins to match expensive workstations and supercomputers, the evaluations on PCs were continuously made. Today almost every software for chemical computation regards PCs running Linux[1] and/or FreeBSD[2] as one of the primary supported platforms.

An attempt of doing computational chemistry on PC systems was reported in 1996 with molecular modeling by Jorgensen et al.[3] The benchmark for electronic structure calculations including ab initio and density functional theories (DFT) with GAUSSIAN 94 revision D.2 was done by Yu and Yu[4] on Intel Pentium and PentiumPro machines running Linux and FreeBSD operating systems. The possibility of improvement by an optimized native FORTRAN compiler designed for the corresponding hardware was proposed. Nicklaus et al.[5] did benchmark for more Linux systems including both ×86 and Alpha machines and suggested that expensive optimization options by the compilers could deliver more performance advantage than the motherboard variations. Since in 1998 the only motherboard chipset available for their target Intel PentiumPro CPU was the Intel LX chipset, the performance of different motherboards hardly differed. Several new competitors in the chipset market, such as VIA Technologies Inc. and Silicon Integrated Systems Corporation(SiS), have offered alternative chipsets which perform no worse than the native chipsets shipped by the CPU manufacturers. Benchmarks done for commercial softwares have shown varied performance from different chipsets,[6] and therefore it becomes obviously important to choose among assorted specifications.

The FORTRAN language is one of the most widely used programming languages for scientific computing. For scientists, it is regarded as a *sine qua non* computer language in addition to the C language. On Linux systems, the earliest FORTRAN interface was the **f2c** translator,[7] which converts FORTRAN to C followed by compilation with the GNU C compiler, **gcc**. The GNU FORTRAN Project, **g77**, integrates the C and FORTRAN compilers. The **g77** is "a program to call **gcc** with options to recognize programs written in FORTRAN (ANSI FORTRAN77, also called F77); **gcc** processes input files through one or more of four stages: preprocessing, compilation, assembly, and linking", quoted from its manual.[8] Therefore **gcc** is viewed as the backend compiler of the **g77** front-end. Many packages in Linux written by FORTRAN use either **f2c** or **g77** as their default FORTRAN compilers. For example, GAUSSIAN 94 used **f2c** as the FORTRAN compiler in its D.2 revision; **g77** is still the default FORTRAN compiler for GAMESS 2000 US version[9] and the MOLPRO 2000 package.[10]

Varieties of other commercial FORTRAN compilers on Linux have been developed to incorporate new FORTRAN90 and FORTRAN95 language extensions as well as the support for parallel and distributed processing. Optimizations for hardware-specific features have been involved to generate performance-oriented executables. For instance, the high-performance FORTRAN products from the Portland Group Inc. (PGI), **pgf77** and **pgf90**, offer tuning options which activate the architectural optimizations for different models

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of CPUs, for instance, the "-tp p5", "-tp p6", "-tp piv", and "-tp athlon" options for the Intel Pentium, Pentium Pro/II/III, Pentium 4, and AMD Athlon processors, respectively. Using this PGI compiler, specification of cache-tiling optimization by the vectorizer at the compiling stage is also possible with designated level-2 (L2) cache size. The newly released Intel FORTRAN compiler (**ifc**) also offers likewise "-tpp5", "-tpp6", and "-tpp7" options to do architectural optimization for Pentium, Pentium Pro/II/III, and especially the Pentium 4 processors.

One of the instruction sets to accelerate floating-point (FP) operations supported by the ×86 processors is Streaming SIMD (single-instruction, multiple data) Extension, commonly known as SSE. The first SIMD instruction set introduced by Intel was its 57 MMX integer (INT) instructions. AMD later implements its first albeit partial SSE support for FP operations into the K6-II processors and has named it as "3DNow!". The Athlon processors with "Thunderbird" core also come with this "3DNow!" support. Lately AMD complies with full-SSE support in the AthlonXP processors with "Palomino" core and terms it as "3DNow! Professional". The SIMD is a limited vector scheme permitting a single operation to proceed with two or four element vectors instead of simple scalar data.[11] The SSE introduces eight 128-bit (four times of 32 bit-wide) single-precision packed CPU registers, enabling the simultaneous computation of four single-precision FP variables. Meanwhile, Intel has launched the second-generation set of SSE (SSE2) for the Pentium 4 CPU. The SSE2 has the capability to handle two 64-bit SIMD INT operations at the same time as well as two element double-precision (also 64-bit) FP vectors or four element single precision vectors. However, the IEEE double-precision FP is 80-bit in precision; therefore, certain technical reviewers have doubts on the competence of the less accurate 64-bit SSE2 FP that aims to replace IEEE double-precision FP in scientific computations.[12] Since the electronic structure calculations employ double-precision FP operations and hence the SSE has little function, the SSE2 has the potential to offer performance advantage. However, the compilers are required to have the SSE2 support, while the source codes may need to be both reprogrammed and recompiled.

Electronic structure calculations involve a huge amount of matrix operations, especially the post-Hartree−Fock methods. Thus the optimized system mathematical libraries for linear algebra can substantially improve the performance. The essential accelerative requirement is the Basic Linear Algebra Subprograms (BLAS),[13−17] which consists of three levels: BLAS1 (vector−vector operations), BLAS2 (vector−matrix operations), and BLAS3 (matrix−matrix operations). Many commercial Unix systems offer libraries tuned for the native processors alone with the operating system libraries or the compilers. The examples are the IRIX of Silicon Graphics Inc. (SGI) and HP-UX of Hewlett-Packard, who ship their own optimized system BLAS libraries with the compilers. Other vendors, like Compaq and IBM, enclose the BLAS libraries within the Digital eXtended Math Library (DXML, renamed to CXML by Compaq)[18] and the Engineering and Scientific Subroutine Library (ESSL),[19] respectively, for Alpha machines running Tru64 Unix or Alpha-Linux and for RS/6000 workstations equipped with AIX. However, these vendor-tuned libraries are not available under the Linux environment; the BLAS library[20] from NETLIB[21] acts as an alternative, which needs installing by system administrators.

The Automatically Tuned Linear Algebra Software (ATLAS)[22] presents very powerful optimized implementation over the three levels of BLAS routines. This library is an application that combines architecture-specific tuning with empirical methods. Traditionally architectural optimization for a given subroutine requires hand-tuning, as certain optimization that improves the performance on one processor may negatively affect the efficiency on another processor.[23] Several discussions on successful speed-up of chemical computations with ATLAS library have been reported on the mail-list of Computational Chemistry List (CCL).[24]

In this benchmark paper, the performance improvements on Linux systems attained by FORTRAN compilers with architectural optimizations as well as the influence of the extensively tuned native libraries are presented. The **pgf77** compiler together with the **ifc** compiler are used with their architectural optimization options for different CPUs to compile the software. The ATLAS library is linked against the executables to replace the untuned BLAS library. The target electronic structure package for the tests is GAUSSIAN 98 revision A.11.[25]

However, it should be particularly addressed that this work only aims for the analyses of tuning potential peak performance on different combinations of hardware, operating systems and compilers, which is similar to the benchmark done by hardware providers with the industrial standard benchmark packages.[26] This experimental action is neither a recommendation nor encouragement to other users to proceed in the same manner in the productive calculations for scientific research whereas nonstandard configurations are unsupported by the software vendor and might lead to ambiguous results of computations without intensive examinations.

SYSTEM DETAIL

The hardware specifications and software environment configurations of the tested platforms are listed in Table 1 as well as the SpecFP2000 base and peak results of the SPEC CPU2000 benchmark suite.[26] These SpecFP2000 values for our PC systems are estimated by the results published on the SPEC Website with the most similar hardware configurations, considering the CPU model and frequency ratio as well as memory types and motherboard chipsets. The SPEC values of TB1 system are estimated by the frequency ratio (1400/1333) to the system equipped with an Athlon 1.3GHz CPU and PC133 SDRAM on the ASUS A7V motherboard (VIA KT133 chipset) running 266 MHz of Front-Side Bus (FSB). The values of the XP1A are estimated by the frequency ratio (1333/1466) to the SPEC system equipped with an AthlonXP 1.466GHz CPU and DDR266 (PC2100 DDR SDRAM) on the EPOX 8KHA+ (VIA KT266A chipset) running 266 MHz FSB. The values of the TB2 system (Tyan S2460 motherboard with AMD 760MP chipset) are copied from the SPEC results by an Athlon 1.4GHz system with DDR266 and Gigabyte GA-7DX motherboard (AMD761 chipset), because the AMD760MP chipset consists of AMD762 as the northbridge.

The new AthlonMP and AthlonXP utilize the same "Palomino" core; therefore, the single-processor performance

Table 1. Hardware Specifications and the Software Configurations of the Tested AMD Athlon Systems in Detail

system name	TB1	TB1A	XP1A	XP1N	TB2	TBMP2	XP2
CPU type[a]	Athlon	Athlon	AthlonXP	Athlon	Athlon	AthlonMP	AthlonXP
L1 cache size	64kB(I) + 64kB(D)	64kB(I) + 64kB(D)	64kB(I) + 64kB(D)	64kB(I) + 64kB(D)	64kB(I) + 64kB(D)	64kB(I) + 64kB(D)	64kB(I) + 64kB(D)
L2 cache size	256 kB	256 kB	256 kB	256 kB	256 kB	256 kB	256 kB
CPU freq	1.4GHz	1.4GHz	1.333GHz	1.4GHz	1.4GHz	1.2GHz	1.4GHz
no. of CPU	1	1	1	1	2	2	2
motherboard	Asus A7V133	MSI K7T266PRO2	MSI K7T266PRO2	MSI K7N420PRO	Tyan S2460	Tyan S2460	Tyan S2460
M/B chipset	VIA KT133A	VIA KT266A	VIA KT266A	nVIDIA nForce420	AMD 760MP	AMD 760MP	AMD 760MP
RAM size	768 MB 256MB×3	512 MB 256MB×2	512 MB 256MB×2	512 MB 256MB×2[b]	512 MB 256MB×2	2048 MB 512MB×4	2048 MB 512MB×4
RAM type	PC133 SDRAM	DDR266 SDRAM	DDR266 SDRAM	DDR266 SDRAM	DDR266 SDRAM	DDR266 ECC Registered	DDR266 ECC Registered
theoretical bandwidth	1066MB/s	2133MB/s	2133MB/s	4266MB/s	2133MB/s	2133MB/s	2133MB/s
OS version	Linux 2.4.10	Linux 2.4.10	Linux 2.4.10	Linux 2.4.10	Linux 2.4.10	Linux 2.4.10	Linux 2.4.10
C compiler	gcc 2.95.4	gcc 2.95.4	gcc 2.95.3	gcc 2.95.4	gcc 2.95.3	gcc 2.95.3	gcc 2.95.3
FORTRAN	PGI/IFC[c]	PGI/IFC	PGI/IFC	PGI/IFC	PGI/IFC	PGI/IFC	PGI/IFC
Math Library	BLAS/ATLAS	BLAS/ATLAS	BLAS/ATLAS	BLAS/ATLAS	BLAS/ATLAS	BLAS/ATLAS	BLAS/ATLAS
SpecFP2000[d]	365/393[e]	426−510/458−549[e]	510/549[e]	N/A	426/458[e]	433/481	483/526[e]

[a] All of the Athlon (with "Thunderbird" core), AthlonMP, and AthlonXP (with "Palomino" core) CPUs of AMD are socket 462 (socket A) and operating at 266 MHz Front Side Bus(FSB). [b] The DIMM1 and DIMM3 of the memory banks on the MIS K7N420PRO are filled to enable the maximum bandwidth of the dual-channel DDR. [c] PGI: Portland Group Inc. FORTRAN Compiler v3.2−4 for Linux; IFC: Intel FORTRAN Compiler v5.0.1, Build 010730D for Linux. [d] SpecFP2000 base/peak values published on the SPEC Website http://www.spec.org. [e] Estimated by the CPU clock ratios to other published benchmark values using the most similar hardware. Described in the SYSTEM DETAIL section.

Table 2. Hardware Specifications and the Software Configurations for the Intel Pentium 4, Alpha, and SGI Systems in Detail

system name	P41.8G	Alpha500	Alpha667	SGI
CPU type	Pentium 4[a]	Alpha 21264A	Alpha 21264A	MIPS R12000
L1 cache size	12kμop(T) + 8kB(D)	64KB(I) + 64KB(D)	64KB(I) + 64KB(D)	32kB(I) + 32kB(D)
L2 cache size	256 kB	4MB	4MB	8MB
CPU freq	1.8GHz	500 MHz	667 MHz	400 MHz
no. of CPU	1	2	2	48
motherboard	Abit TH7II	API DP264	API DP264	Origin 3800
M/B chipset	Intel i850	Compaq 21272	Compaq 21272	
RAM size	1024 MB 256MB×4[b]	2048 MB 128MB×16[b]	2048 MB 128MB×16[b]	48GB
RAM type	PC800 RAMBUS	83 MHz SDRAM 256 bit Bus, 72bit ECC	83 MHz SDRAM 256 bit Bus, 72bit ECC	
theoretical bandwidth	3200MB/s	2650MB/s	2650MB/s	3.2GB/s
OS version	Linux 2.4.10	Tru64 v4.0F	Tru64 v4.0F	IRIX 6.5
C compiler	gcc 2.95.3	DEC C V5.9−010	DEC C V5.9−010	MIPSpro 7.3.1.2m
FORTRAN	PGI/IFC[c]	Digital Fortran v5.2	Digital Fortran v5.2	MIPSpro 7.3.1.2m
Math Library	BLAS/ATLAS	DXML(CXML)	DXML(CXML)	System BLAS
SpecFP2000[d]	669/678	383/422	<514/577[e]	382/407

[a] The Pentium 4 CPU is socket 478 (with "Willamette" core) and operating at 400 MHz FSB. [b] All the memory banks of the Pentium 4 and Alpha systems are filled to accomplish maximum bandwidth due to the dual-channel and switched buses. [c] PGI: Portland Group Inc. FORTRAN Compiler v3.2−4 for Linux; IFC: Intel FORTRAN Compiler v5.0.1, Build 010730D for Linux. [d] SpecFP2000 base/peak values published on the SPEC Website (http://www.spec.org). [e] The marks should be lower than the Compaq DS20E/667 MHz system with 8MB of L2 cache.

on the same motherboard should be identical, and the SpecFP2000 value of the dual-AthlonXP on Tyan S2460 is taken from the system of dual-1.4G AthlonMP with Tyan ThunderK7. Other published SpecFP2000 results have the entries of the AthlonMP 1.2GHz on Tyan ThuderK7, the Intel Pentium 4 1.8GHz with Intel i850 chipset, and the SGI Origin system with MIPS R12000 400 MHz CPU, and therefore these values are reproduced into Table 1. For our Alpha machines, they employ the identical motherboard (API DP264) to the Compaq DS20/DS20E systems with 21264A 500 MHz and 667 MHz CPUs; the only difference is the L2 cache size (4MB v.s. 8MB). The SPEC results of those Compaq systems are henceforth used in Tables 1 and 2. No hardware similar to the TB1A system is available on the SPEC report, but it should range between TB2 and XP1A. These values may not be exact due to other factors such as operating systems and compilers but regardless can provide a preliminary reference of the CPU performances.

The Linux distributions that are installed include Slackware[27] 8.0 (with **gcc** 2.95.3) and Debian[28] GNU/Linux3.0 ("Woody" release, with **gcc** 2.95.4). All the systems have been upgraded to kernel version 2.4.10, whose drivers for the motherboard chipsets, namely the VIA KT133A, VIA KT266A, AMD 760MP and Intel i850, are all enabled. The memory banks of the Pentium 4 system (4 banks) and the Alpha systems (16 banks) are exclusively filled to enable the maximum memory bandwidth by their dual-channel RAMBUS and crossbar switching architectures, respectively. The DIMM1 and DIMM3 memory banks of XP1N are filled to utilize full bandwidth of dual-channel double-data rate (DDR) memory.

Table 3. Detailed Description of Each Job Selected for Benchmark

test	molecular stoichiochemistry and symmetry	theory	basis set	NBF[a]	job type	remark
322−1	C_{60} (I_h/C_{2h})	RHF	STO-3G	300	optimization	
322−2					frequency	
322−3					frequency	numerical
338	neopentane C_5H_{12} (D_2)	RB3LYP	6-31G(df,dp)	242	optimization	
339	$Na(H_2O)_4^+$ (S_4)	RB3LYP	6-31G(df,dp)	202	optimization	
364	$C_{20}H_2O$ (C_{2h})	RHF	6-311G**	480	single point	SCF=tight
397	valinomycin $C_{54}H_{90}N_6O_{18}$ (C_1)	RB3LYP	3-21G	882	force	
415−1	fluoroethylene CH_3CH_2F (C_s)	RMP2/full	6-311G(df,dp)	108	single point/	molecule
415−2		UMP2/full			NMR	cation
420−1	trimethylsilylacetylene	RMP2/FC[b]	6-311G(2df,p)	248	single point	
420−2	$C_5H_{10}Si$ (C_3)				single point	full int sort
424−1	toluene C_7H_8 (C_s)	RMP2/FC	6-31G*	114	frequency	
424−2					frequency	full int sort
438	C_{14} (D_{7h}/C_{2v})	RB3LYP-TD	6-31G(d)	210	single point	10 states
439−1	fluoradenide $C_{19}H_{11}$ (C_{2v})	RHF	6-31+G*	383	optimization	
439−2					frequency	
447−1	$Ca(C_5H_5)^+$ (C_s)	MPW1PW91	6-311+G*	168	optimization	
447−2					frequency	
559−4	water dimer counterpoise (C_s)	RHF	3-21G	26	frequency	energy only
560−4	water dimer counterpoise (C_s)	RMP2/FC	3-21G	26	frequency	energy only
561−4	water dimer counterpoise (C_s)	RB3LYP	3-21G	26	frequency	energy only

[a] Number of the basis functions. [b] Frozen-core MP2.

BENCHMARK SETUP

One of the most frequently used packages for electronic structure calculation is GAUSSIAN 98(G98).[25] In the benchmark for G98, we use the standard test-files included within this package. To make meaningful comparisons for the CPU usage, only the jobs consuming ostensive CPU time are considered. Three types of computations that are the most frequently performed: the geometrical optimization, the single point energy, and the vibrational frequency calculation, are chosen. These selected test-files are listed in Table 3 and in detail described with the levels of theories, the basis sets, the number of basis functions, and the calculation types. The theories include Hartree−Fock (HF) and DFT as well as the second-order Møller Plesset theory (MP2). On Linux systems, the default FORTRAN compiler to make the G98 is the **pgf77** compiler of Portland Group Inc.[29] The Intel FORTRAN compiler (**ifc**),[30] which is assumed to be the "native compiler" for the Intel CPUs, is also used to compile G98; the **ifc** has a very similar style of optimization options to **pgf77**. Two mathematical libraries, the BLAS library included in the G98 package as well as the ATLAS library, are linked respectively, against G98 to compare the performance improvement. For the **pgf77** compiler, tuning options "-tp p6" and "-tp athlon" are exclusively tested to judge the architectural optimization improvement over the AMD Athlon series processors. Likewise, for the Intel Pentium 4 system, we have tried the "-tp p6" and "-tp piv" options by **pgf77** as well as the "-tpp6" and "-tpp7" options by **ifc**. In addition, the default optimization options to **pgf77** other than these architectural optimizations set by G98 are "-Munroll -Mvect = cachesize:**L2-cache-size**" and are retained. The relative optimization options to **ifc** except the architectural optimization are therefore set to "-unroll" only, being consistent with **pgf77**. The optimization level "-O#", where # = 0, 1, or 2, for each subroutine is specified as the default setting in the original makefile (i386.make).

The ATLAS library employed is version 3.2.1 for all the PC systems except that on the Pentium 4 machine, where version 3.3.7D is installed to have the SSE2 support. The various architectural optimization options offered by the two distinct FORTRAN compilers mentioned in the preceding paragraph, however, are not specified while compiling the ATLAS library since ATLAS mainly relies on the C compiler. The only FORTRAN routines in ATLAS library are the interface routines of FORTRAN77, which are not responsible for computation. The FORTRAN compilers therefore have no effect on the performance.[31] The C compiler used on all Linux systems is **gcc** version 2.95 series. All the jobs run with single CPU even though on some systems more than one CPU are installed.

RESULTS AND DISCUSSION

The benchmark results are shown in Tables 4−7. All of the selected tests on Linux systems were unsuccessful for the second part of test415 due to the constraint of file-size. The largest file-size that the 32-bit Linux machines can address is 2 GB. Although the Linux kernel version 2.4 can handle large files, merely specifying the "-D_FILE_OFFSET_BITS = 64" flag[32] with the **gcc** would not only fail to enable large-file support but would also render all the binaries defunct. The practical solution to this limitation is to split the RWF file into several files less than 2GB. The executables compiled by **ifc** with solely architectural optimizations are observed to abnormally terminate for test364 due to an unknown address error; however, specifying the vectorization (-axK and -axW) solves this problem.

Mathematical Libraries. For all PC-Linux systems, the imposition of the ATLAS library does not show significant improvements over the Hartree−Fock calculations, namely test322, test338, test339, and the second part of test415 as well as the small-size frequency calculations in test559, test560, and test561 which only has 26 basis functions. For DFT methods, hybrid-type B3LYP obtains no acceleration by ATLAS over the geometrical optimization jobs. However, linking against the ATLAS library does not obstruct the performance either. Yet for the post-Hartree−Fock calculations such as MP2, employing the ATLAS library can obviously accelerate the speed, especially for the gradient

Table 4. CPU Time that Each Test Job Consumes on Single-CPU AMD Athlon and AthlonXP Systems[f]

system	G98[a]	TB1						TB1A				XP1A							
compiler arch. opt.[b] library		pgf77 -tp p6 BLAS	pgf77 -tp p6 ATLAS	pgf77 -tp athlon BLAS	pgf77 -tp athlon ATLAS	ifc -tpp6 BLAS	ifc -tpp6 BLAS	pgf77 -tp p6 BLAS	pgf77 -tp p6 ATLAS	ifc -tpp6 BLAS	ifc -tpp6 ATLAS	pgf77 -tp athlon BLAS	pgf77 -tp athlon ATLAS	ifc -tpp6 BLAS	ifc -tpp6 ATLAS	ifc (a) BLAS	ifc (a) ATLAS	ifc (b) BLAS	ifc (b) ATLAS
322-1	5.17	8.75	8.46	8.76	8.48	7.08	7.06	7.36	7.17	5.82	5.86	6.48	6.38	5.30	5.38	5.26	5.30	5.28	5.29
322-2	142	167	166	166	166	115	116	149	150	99	100	142	142	94	94	94	93	95	94
322-3	236	305	304	305	305	203	203	276	275	176	177	253	153	164	165	163	163	164	163
338	35	55	51	55	51	39	37	49	46	33	32	40	37	30	28	30	28	30	28
339	44	56	54	56	54	40	39	51	49	34	34	44	36	32	31	32	31	32	31
364[e]	44	41	42	42	42	*c*	*c*	39	39	*c*	*c*	36	36	*c*	*c*	*c*	*c*	26	26
397	684	843	841	844	839	619	614	734	728	519	513	610	608	479	478	478	477	473	473
415-1	29	37	31	37	31	30	25	33	27	25	21	29	25	23	20	23	20	23	20
415-2[e]	62	*d*	*d*	*d*	*d*	*d*	*d*	*d*	*d*	*d*	*d*	*d*	*d*	*d*	*d*	*d*	*d*	*d*	*d*
420-1	131	198	181	197	180	154	141	168	157	128	119	150	135	118	109	118	109	118	109
420-2	153	198	181	197	181	155	141	172	159	128	118	150	136	118	109	118	109	118	109
424-1	89	145	89	145	89	113	74	120	77	91	–	109	71	86	59	86	59	85	59
424-2	89	145	89	145	89	113	74	120	77	91	–	109	71	86	59	86	59	85	59
438	52	60	52	60	52	50	42	55	47	45	40	52	41	43	34	43	34	43	34
439-1[e]	134(2)	299(4)	164(2)	298(4)	164(2)	112(2)	112(2)	267(4)	148(2)	97(2)	93(2)	244(4)	135(2)	92(2)	92(2)	92(2)	92(2)	165(4)	91(2)
439-2	102	124	123	124	124	85	85	111	111	73	73	102	105	70	70	70	70	69	71
447-1	194	322	278	322	278	233	200	289	250	197	174	229	196	177	154	177	154	175	155
447-2	116	159	143	157	143	118	106	144	131	105	93	118	103	93	80	93	79	93	80
559-4	31	26	26	26	26	19	19	19	19	14	13	19	19	13	13	13	13	13	13
560-4	35	30	30	30	30	21	21	23	23	15	15	22	22	15	15	15	15	15	15
561-4	81	61	60	61	60	48	48	52	52	41	41	53	52	42	42	42	42	41	41
sum	2248	2940	2707	2936	2706	2162	1992	2572	2385	1820	–	2237	1958	1688	1565	1686	1560	1677	1559

[a] The CPU time in the g98 packages under $g98root/g98/tests/sgi directory. [b] The optimization to **ifc** other than the architectural optimization is set to "-unroll -O2". [c] Bump out due to unknown address error reported by **ifc.** [d] Error due to failure to write scratch files larger than 2 GB. [e] Excluded from sum. [f] The unit of the CPU time is in minutes; the numbers in the parentheses are the step numbers required in the geometrical optimization calculations: (a) -tpp6 -ipo -ipo_obj and (b) -tpp6 -axK -ipo -ipo_obj.

Table 5. CPU Time that Each Test Job Consumes on Single-CPU AMD Athlon and AthlonXP Systems[e]

system	XP1N								XP2									
compiler arch. opt.[a] library	pgf77 -tp athlon BLAS	pgf77 -tp athlon ATLAS	ifc -tpp6 BLAS	ifc -tpp6 ATLAS	ifc (a) BLAS	ifc (a) ATLAS	ifc (b) BLAS	ifc (b) ATLAS	pgf77 -tpp6 BLAS	pgf77 -tpp6 ATLAS	pgf77 -tp athlon BLAS	pgf77 -tp athlon ATLAS	ifc -tpp6 BLAS	ifc -tpp6 ATLAS	ifc (a) BLAS	ifc (a) ATLAS	ifc (b) BLAS	ifc (b) ATLAS
322-1	5.54	5.46	5.49	4.60	4.48	4.58	4.49	4.57	7.45	7.48	7.51	6.68	6.80	5.77	5.98	6.83	6.08	6.61
322-2	129	129	82	83	83	83	83	83	156	153	150	143	111	96	96	109	103	109
322-3	230	230	144	145	144	144	144	144	284	269	271	256	167	169	194	192	196	197
338	35	33	26	25	26	25	26	25	47	42	46	39	32	30	38	34	38	33
339	39	38	28	27	28	27	28	27	50	46	51	43	33	32	39	35	39	37
364[d]	33	34	*b*	*b*	26	25	24	25	38	37	39	36	*b*	*b*	29	31	29	29
397	536	534	411	409	405	405	405	405	639	707	657	692	598	568	571	608	620	624
415-1	26	22	20	17	20	17	20	17	34	28	34	26	32	25	29	24	29	24
415-2[d]	*c*	*c*	*c*	*c*	*c*	*c*	*c*	*c*	*c*	*c*	*c*	*c*	*c*	*c*	*c*	*c*	*c*	*c*
420-1	128	118	100	93	100	93	100	93	181	135	180	141	134	127	145	141	152	142
420-2	128	118	100	93	100	93	100	93	180	139	173	141	134	129	155	138	156	141
424-1	94	63	73	51	73	51	73	51	140	80	133	72	112	65	111	69	102	65
424-2	94	63	73	51	73	51	73	51	140	81	133	72	112	66	111	67	103	70
438	48	38	39	30	39	30	39	30	57	45	56	41	45	37	48	40	48	40
439-1[d]	223(4)	122(2)	81(2)	81(2)	146(4)	80(2)	146(4)	80(2)	275(4)	154(2)	270(4)	144(2)	119(2)	105(2)	206(4)	108(2)	207(4)	115(2)
439-2	93	92	61	61	61	66	61	66	104	110	114	104	93	70	86	86	85	85
447-1	200	174	152	134	151	134	151	134	246	220	272	231	221	189	231	196	229	194
447-2	107	93	83	70	83	70	83	70	124	115	134	120	115	93	117	98	112	94
559-4	17	17	12	12	12	12	12	12	21	24	25	21	20	20	21	20	21	18
560-4	20	20	13	14	14	14	14	14	24	28	29	24	22	21	23	22	21	23
561-4	49	48	38	38	38	38	38	38	54	58	60	53	50	47	50	50	48	47
sum	1979	1835	1460	1358	1454	1358	1454	1358	2488	2287	2526	2226	2038	1790	2071	1936	2108	1950

[a] The optimization to **ifc** other than the architectural optimization is set to "-unroll -O2". [b] Bump out due to unknown address error reported by **ifc**. [c] Error due to failure to write scratch files larger than 2 GB. [d] Excluded from sum. [e] The unit of the CPU time is in minutes; the numbers in the parentheses are the step numbers required in the geometrical optimization calculations: (a) -tpp6 -axK and (b) -tpp6 -axK -ipo -ipo_obj.

Table 6. CPU Time that Each Test Job Consumes on the Dual-CPU AMD Athlon and AthlonMP Systems[e]

system	TB2						TBMP2					
compiler arch. opt.[a] library	pgf77 -tp p6 BLAS	pgf77 -tp p6 ATLAS	pgf77 -tp athlon BLAS	pgf77 -tp athlon ATLAS	ifc -tpp6 BLAS	ifc -tpp6 ATLAS	pgf77 -tp p6 BLAS	pgf77 -tp p6 ATLAS	pgf77 -tp athlon BLAS	pgf77 -tp athlon ATLAS	ifc -tpp6 BLAS	ifc -tpp6 ATLAS
322-1	9.65	9.08	10.05	8.87	7.48	7.67	8.81	9.37	8.51	8.47	6.85	6.79
322-2	166	165	171	172	114	108	145	179	167	167	110	112
322-3	305	308	305	317	208	192	296	335	312	312	194	198
338	58	57	57	55	42	35	50	47	48	50	37	36
339	57	59	57	57	42	37	54	52	54	55	39	38
364[d]	44	46	44	45	*b*	*b*	43	43	42	45	*b*	*b*
397	848	918	847	862	644	634	748	687	692	775	597	617
415-1	40	36	40	34	34	27	51	38	44	44	33	33
415-2[d]	*c*	*c*	*c*	*c*	*c*	*c*	*c*	*c*	*c*	*c*	*c*	*c*
420-1	206	195	198	192	161	139	208	188	184	197	163	150
420-2	199	187	198	191	160	139	208	184	184	200	173	148
424-1	161	92	161	94	130	75	179	104	142	106	140	87
424-2	161	95	161	93	131	75	176	104	142	102	145	85
438	61	55	61	53	53	42	60	50	59	51	56	41
439-1[d]	297(4)	190(2)	297(4)	175(2)	116(2)	111(2)	286(4)	166(2)	274(4)	164(2)	128(2)	114(2)
439-2	123	131	123	123	86	83	120	126	115	126	92	89
447-1	339	295	340	289	248	202	299	229	266	248	224	207
447-2	165	153	163	156	125	112	146	119	136	128	116	104
559-4	21	23	21	21	14	16	29	23	23	26	19	20
560-4	25	27	24	24	16	19	33	27	27	30	21	21
561-4	56	58	55	55	46	47	66	61	61	65	52	52
sum	3001	2863	2992	2797	2261	1990	2877	2562	2665	2690	2218	2045

[a] The optimization to **ifc** other than the architectural optimization is "-unroll -O2". [b] Bump out due to unknown address error reported by **ifc**. [c] Error due to failure to write scratch files larger than 2 GB. [d] Excluded from sum. [e] The unit of the CPU time is in minutes; the numbers in the parentheses are the step numbers required in the geometry optimization calculations.

Table 7. CPU Time that Each Test Job Consumes on the Intel Pentium 4, Alpha, and SGI Systems

system	P41.8G												Alpha500	Alpha667	SGI
compiler arch. opt.[a] library	pgf77 -tp p6 BLAS	pgf77 -tp p6 ATLAS	pgf77 -tp piv BLAS	pgf77 -tp piv ATLAS	ifc -tpp6 BLAS	ifc -tpp6 ATLAS	ifc -tpp7 BLAS	ifc -tpp7 ATLAS	ifc (a) BLAS	ifc (a) ATLAS	ifc (b) BLAS	ifc (b) ATLAS	f90 -tune ev6 DXML	f90 -tune ev6 DXML	f77 -mips4 -rl0000 system blas.a
322-1	4.25	4.46	4.23	4.55	3.39	3.69	3.38	3.65	3.21	3.56	3.22	3.53	7.87	6.37	5.47
322-2	127	130	127	128	77	77	78	78	75	75	74	74	154	136	158
322-3	192	193	192	196	127	127	126	126	127	127	125	125	225	202	265
338	31	31	31	31	23	22	22	22	22	22	22	21	36	32	42
339	35	35	35	35	25	25	25	25	24	24	24	24	43	39	53
364[f]	44	44	44	44	*b*	*b*	*b*	*b*	30	31	30	31	48	39	53
397	487	487	485	487	363	366	363	362	341	339	339	338	658	602	737
415-1	19	17	19	17	16	14	16	14	15	14	15	13	24	21	33
415-2[f]	*c*	*c*	*c*	*c*	*c*	*c*	*c*	*c*	*c*	*c*	*c*	*c*	52	46	71
420-1	91	88	92	90	74	69	73	69	71	68	71	68	113	107	156
420-2	92	88	92	88	74	70	73	69	72	73	72	69	136	128	188
424-1	61	49	61	49	52	41	52	41	47	39	47	39	76	65	98
424-2	61	49	61	49	52	41	52	40	47	39	47	40	75	65	98
438	44	34	43	32	39	27	38	27	27	26	28	26	75	64	58
439-1[f]	188(4)	109(2)	185(4)	109(2)	72(2)	71(2)	71(2)	71(2)	69(2)	*d*	68(2)	*d*	123(2)	111(2)	156(2)
439-2	79	79	79	80	55	55	54	55	47	51[e]	47	51[e]	90	81	121
447-1	171	161	171	161	129	120	127	118	122	116	122	114	214	191	215
447-2	94	80	93	79	77	63	77	63	65	59	65	58	121	104	153
559-4	16	16	16	16	11	12	11	11	11	10	11	10	35	31	155
560-4	19	19	19	19	13	13	13	13	12	12	13	12	40	36	152
561-4	54	54	54	54	38	38	38	38	35	35	35	35	90	95	201
sum	1677	1614	1674	1616	1248	1184	1241	1175	1163	1133	1160	1121	2213	2005	2888

[a] The optimization to **ifc** other than the above architectural optimization is "-unroll -O2". [b] Unknown address error reported by **ifc**. [c] Error due to failure to write scratch files larger than 2 GB. [d] Geometrical optimization did not converge. [e] Restarted by a converged structure. [f] Excluded from sum. [g] The unit of the CPU time is in minutes; the numbers in the parentheses are the step numbers required in the geometry optimization calculations: (a) -tpp7 -axW and (b) -tpp7 -axW -ipo -ipo_obj.

calculations as vibrational frequencies; the best case is test424, which receives about 40% speed-up by ATLAS using both FORTRAN compilers on Athlon systems. For DFT frequencies the speed-up is around 5%. For time-dependent DFT (TD-DFT) calculations, the acceleration varies with compilers. The **ifc** delivers a 20% enhancement, while **pgf77** only archives 13%. Furthermore, the improvement made by ATLAS is comparably smaller on Pentium 4 (P4) than those on the Athlon systems (13%).

The ATLAS library either improves the execution speed providing exactly the same results or decreases the step numbers required to converge geometrical optimization by a few digits of variations: for the geometrically optimized Hartree−Fock energy of the first part of test439, Alpha =

−725.9409551 (2 steps), SGI = −725.9409068 (2 steps); P4+**pgf77** + BLAS = −725.9409038 (4 steps), P4 + **pgf77** + ATLAS = −725.9409551 (2 steps), P4 + **ifc** + BLAS = −725.9409551 (2 steps), and P4 + **ifc** + ATLAS = −725.9409551 (2 steps); Athlon + **pgf77** + BLAS= −725.9409038 (4 steps), Athlon + **pgf77** + ATLAS = −725.9409551 (2 steps), Athlon + **ifc** + BLAS = −725.9409551 (2 steps), and Athlon + **ifc** + ATLAS = −725.9409068 (2 steps); all in atomic units. Additionally, the instability of acceleration by ATLAS is observed on the dual-Athlon systems, even though only a single processor is actually employed.

Compiler Options: (i) Architectural Optimizations. Since **ifc** is a relatively new compiler supporting FORTRAN77 and FORTRAN90 as well as FORTRAN95 extensions, several command-line parameters are required to compile codes consisting of old FORTRAN styles. The option "-WB" must be specified to disable the out-of-bound array checking by default. Various comment messages and warnings of using nonstandard FORTRAN can be suppressed with the options of "-cm" and "-w", respectively. To coexist with C language, the Intel FORTRAN I/O library archived in **libCEPCF90.a** may be invoked at the linking stage by the option of "-Vaxlib". Other commonly employed but undefined references in **ifc,** such as forking and termination waiting for child processes, need to be defined by hand.

The **ifc** generally makes G98 run faster than **pgf77**; even on AMD Athlon systems, **ifc** with "-tpp6" option can accelerate G98 much more than **pgf77** with "-tp athlon" option. For **pgf77** on Athlon systems, the architectural optimization "-tp athlon" produces insignificant speedup compared to the option "-tp p6". Worse, it occasionally caused unsteady performance in several cases on dual-Athlon configurations, for example, the slow-down for test559, test560, and test561 on XP2 system with BLAS library. On Pentium 4 systems, **pgf77** with "-tp piv" option hardly improves the performance compared to "-tp p6" option. Therefore it is concluded that "-tp p6" may be the most suitable universal architecture optimization option for any processors with **pgf77**.

(ii)Vectorization for SSE and SSE2. It is noticeable that on the Pentium 4 system, the ATLAS library v3.3.7 is supposed to utilize the SSE2 support. However, in Table 7, when we compare the results of test420, which consist of MP2 calculations with the most basis functions (248) among our tests, it is found using both compilers with ATLAS displays no more significant speed-up than using solely the BLAS library (**pgf77**: 4% v.s. **ifc**: 5%), and therefore it is suggested that **pgf77** with "-tp piv" and **ifc** with "-tpp7" only has not activated the SSE2 instruction sets.

In the documentation of the **pgf77** compiler, there is an option "-Mvect=sse" to enable the SSE support for the Intel Pentium III and the capable "3DNow!" instruction set of the AMD Athlon CPUs. The corresponding activations for **ifc** are "-axK" and "-axW", respectively, for SSE and SSE2 instructions. In Table 4 we observe that the "-axK" option has no performance advantage over the optimization, which indicates that single-precision SSE instruction sets offer no performance improvement over the double-precision floating-point computations that are used in the electronic structure calculations. The only use of this vectorization is to eliminate certain address errors which occurred in test364. In Table 7, it is proved that "-axW" option can initiate the SSE2 support on the Pentium 4 system and further more accelerates the large-size computations. Nevertheless, this may involve several precision problems cooperating with the ATLAS library and hence fail to converge the geometrical optimization tasks as in test439.

(iii) Interprocedural Optimization. The **ifc** compiler offers the "-ipo" option which enables multifile interprocedural optimizations between source files. The option "-ipo_obj" must be specified simultaneously with "-ipo" to force the generation of real object files while compiling G98 in order to link against the BLAS and ATLAS libraries. This optimization takes very expensive compilation time but has hardly any improvement over the speed of G98.

In conclusion, the best architectural tuning options of **ifc** on Intel Pentium 4 system are "-tpp7 -axW" for G98. For single-Athlon system, the optimal architectural optimization would be "-tpp6 -axK". For dual-Athlon systems using AMD 760MP chipset the proper architectural tuning should be "-tpp6 -axK". Although using the "-axK" option has caused instable speed enhancement on dual-Athlon systems, it cannot be omitted to prevent from certain unknown address error occurred in test364. All these architectural options combining with "-O2 -unroll" optimization would make the best single-processor performance for G98 on Linux systems.

SpecFP2000 Benchmark. Since all of the system vendors have done their best to tune their own systems for the SPEC benchmark, the published values and corresponding environments are the optimal condition on each machine. The Compaq DS20/500 system with 4MB L2 cache on the SPEC list[33] running Tru64 Unix V4.0F and Digital FORTRAN v5.3 shows a SpecFPBase2000 mark of 383 and only differs in minor revisions of the compiler compared to our Alpha500 system. Therefore we compare our benchmark results of the PC systems to this Alpha500 machine and further analyze the relation of the best FP performance between the SpecFP2000 and the G98 package in Table 8. As the SpecFPBase2000 mark for the XP1A systems is 510, we then obtain the multiplier of 1.33 (383 divided by 510) in the SpecFPBase2000 mark. The summation of CPU time over all the tests except test364, the second part of test415, and the first part of test439 consumed on the XP1A system is 1565 min, while these tests took 2213 min on the Alpha500 system, resulting in a speed factor of 1.41. If the native Digital FORTRAN compiler with DXML library has done the best FP optimization over the Alpha500 system, so has **ifc** with ATLAS achieved on XP1A because the quotient of G98 speed is larger than that of SpecFPBase2000. Similarly, comparing the TBMP2 and XP2 systems to the Alpha500 machine, the relative speeds of G98 are 1.08 and 1.24, respectively, while the ratios of the SpecFPBase2000 mark are 1.13 and 1.26. In addition, based on the SpecFPBase2000 points the P41.8G system gained 669 marks, which is measured on an Intel 1.8GHz Pentium 4 system running Microsoft Windows2000 Service Pack 2 with Intel FORTRAN compiler v5.0.1 for Windows, base tuning options being "-Qipo -QxW -O3".[34] As aforementioned the SpecFPBase2000 mark for the Alpha500 system is 383, the P41.8G system is supposed to be about 1.75 times faster than Alpha500. Summing up the CPU time of G98 benchmark for P41.8G with the combinations of [**ifc** -tpp7 + BLAS], [**ifc** -tpp7 + ATLAS], and [**ifc** -tpp7 -axW + BLAS], the

Table 8. Performance Correlation between the SpecFP2000 Marks and the Best GAUSSIAN 98 Results on PC-Linux Systems[c]

system name	Alpha500	TB1	XP1A	XP1N	TB2	TBMP2	XP2	P41.8G	P41.8G	P41.8G
FORTRAN compiler	f90	ifc	ifc	ifc	ifc	ifc	ifc	ifc	ifc	ifc
architectural optimizations	-tune ev6 -arch ev6	-tpp6	-tpp6	-tpp6	-tpp6	-tpp6	-tpp6	-tpp7	-tpp7	-tpp7 -axW
numerical library	DXML	ATLAS	ATLAS	ATLAS	ATLAS	ATLAS	ATLAS	BLAS	ATLAS	ATLAS
sum of CPU time	2213	1992	1565	1358	1990	2045	1790	1241	1175	1133
inverse ratio of time	1.00	1.11	1.41	1.63	1.11	1.08	1.24	1.78	1.88	1.95
SpecFP2000 base	383	365[a]	510	624[b]	426	433	483	669	669	669
SpecFP2000 ratio	1.00	0.95	1.33	1.63	1.11	1.13	1.26	1.75	1.75	1.75
SpecFP2000 peak	422	393[a]	549	688[b]	458	481	526	678	678	678
SpecFP2000 ratio	1.00	0.93	1.30	1.63	1.09	1.14	1.25	1.61	1.61	1.61

[a] Estimated by the clock frequency. [b] Estimated by the benchmark results of GAUSSIAN 98. [c] The results obtained on PC-Linux systems are compiled using "ifc -O2 -unroll" with the listed architectural optimization options and linked against corresponding numerical libraries. The summation over CPU time includes all the test-files listed in Table 2 except test364, the second part of test415, and the first part of test439. All ratios are relative to the Alpha500 system.

speed ratios to the Alpha500 system are 1.78, 1.88, and 1.95, respectively. As P41.8G's factor of SpecFPBase2000 mark to Alpha500 is 1.75, it is concluded that full optimizations including the SSE2 functions (by "-axW") have been enabled for G98 with the **ifc** compiler on Pentium 4 systems running Linux; using the ATLAS library its optimal FP performance is superior to that SpecFP benchmark that has been done under the Windows environment.

CONCLUDING REMARK

From the hardware point of view, up-to-date PC systems can be loaded with much more memory than 512MB, the maximum amount a few years ago. Motherboards for a single Athlon with VIA KT266A chipset can address up to 4 GB of registered memory (or 3GB of unregistered RAM), while the Tyan S2460 motherboard for dual-Athlon can support at most 3 GB of memory. As for the Pentium 4, motherboards with Intel i850 chipsets can handle up to 2 GB of memory, while the motherboards for dual-Xeon with Intel i860 chipsets maximally support 4 GB of memory. With the DDR and RAMBUS technologies, these PC systems offer significantly wider memory bandwidths than before, which enable PCs to compete with workstations and to improve the performance for large computations. The instruction set of double-precision floating-point operations is extensively beneficial to the electronic structure calculations. Currently only the SSE2 instructions of Intel Pentium 4 support this. The compatible implementation of this double-precision FP to the next generation of AMD CPU (the "Hammer" core) is anticipated. Larger size of the L2 cache also helps to improve the performance. The next generation of the Intel Pentium 4 (the "Northwood" core) is expected to have 512kB of L2 cache. Nowadays the role of motherboard chipsets, therefore, cannot be overlooked in terms of the performance. Due to our benchmark result, the G98 package demands high memory bandwidth.

In our previous benchmark paper,[4] the slowest calculation on a high-end PC at that time was only one-twelfth of the speed of an SGI PowerChallenge back in 1997; furthermore, we had concluded that an optimized FORTRAN compiler is indispensable for the ultimate improvement on Linux systems. The report by Nicklaus et al.[5] also showed the possibility of acceleration by expensive compiler optimization tuning options. In addition to the progress of the PC hardware, recent developments in the FORTRAN compilers by the hardware originator have achieved a successful stage to do optimizations and therefore exerted full power of the commodity-type microprocessors for large-scale electronic structure calculations; in most cases the desktop PC systems perform as good as or even better than an expensive workstation today. The Intel FORTRAN compiler offers several conditions of free evaluations albeit unsupported[35] and supplies with fine optimization strategies for both native $\times$86 and compatible processors. The efficiency of post-Hartree−Fock calculations can be benefited from the ATLAS library. Therefore the PC-Linux systems have become extremely competitive to the relatively costly workstations and exhibit very high performance for single-processor calculations. Once the large-file constrain is eliminated, most research groups with limited funding can replace other Unix workstations with PC-Linux systems.

The SpecFP2000 benchmark generates pretty good correlation between the FP performance and the real applications. The scaling by the frequency ratio corresponding to the same peripherals is capable of estimating the performance of the same CPU model with different clock frequencies.

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(22) Whatley, R. C.; Petitet A.; Dongarra, J. J. Automated Empirical Optimization of Software and the ATLAS Project, dated Sep. 19, 2001. Download from http://www.netlib.org/lapack/lawns/lawn147.ps. The ATLAS source code can be downloaded from http://math-atlas.sourceforge.net or http://www.netlib.org/atlas.
(23) http://math-atlas.sourceforge.net/faq.html#help.
(24) http://www.ccl.net/chemistry/resources/messages/index.shtml. Established in 1991, the Computational Chemistry List (CCL) is dedicated to fostering communication within the worldwide community of researchers involved in chemistry-focused computation. See http://www.ccl.net.
(25) GAUSSIAN 98 (Revision A.11); M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, V. G. Zakrzewski, J. A. Montgomery, Jr., R. E. Stratmann, J. C. Burant, S. Dapprich, J. M. Millam, A. D. Daniels, K. N. Kudin, M. C. Strain, O. Farkas, J. Tomasi, V. Barone, M. Cossi, R. Cammi, B. Mennucci, C. Pomelli, C. Adamo, S. Clifford, J. Ochterski, G. A. Petersson, P. Y. Ayala, Q. Cui, K. Morokuma, P. Salvador, J. J. Dannenberg, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. Cioslowski, J. V. Ortiz, A. G. Baboul, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. Gomperts, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, J. L. Andres, C. Gonzalez, M. Head-Gordon, E. S. Replogle, J. A. Pople, Gaussian, Inc., Pittsburgh, PA, 2001.
(26) SPEC CPU2000 is the next-generation industry-standardized CPU-intensive benchmark suite. SPEC designed CPU2000 to provide a comparative measure of compute intensive performance across the widest practical range of hardware. See http://www.spec.org/osg/cpu2000.
(27) http://www.slackware.org.
(28) http://www.debian.org.
(29) http://www.pgroup.com/prodworkpgf77.htm.
(30) http://developer.intel.com/software/products/compilers/f50/linux/.
(31) See the *Installing additional f77 interfaces* section of the ATLAS FAQ at http://math-atlas.sourceforge.net/errata.html#MultF77.
(32) Specifying this flag while compiling MOLPRO 2000 can overcome the 2GB limitation.
(33) http://www.spec.org/osg/cpu2000/results/res1999q4/cpu2000-19991130-00010.html.
(34) http://www.spec.org/osg/cpu2000/results/res2001q3/cpu2000-20010827-00817.html. The -QxW option by **ifc** under Microsoft Windows generates specialized code to run exclusively on the Pentium 4 processor supporting its new instruction extensions. Refer to the manual of Intel FORTRAN Compiler.
(35) http://developer.intel.com/software/products/compilers/f50/linux/noncom.htm.

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