

# 64-bit RICS machines in computational chemistry - summary

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## 1 Introduction

This is a summary of all the knowledge about 64-bit machines for computational chemistry I've got so far. Those information has been gathered not only from this list (CCL), but also from Amber's mailing list and from the authors of the computational chemistry codes.

## 2 CC codes

I sent this e-mail to the individual authors of CC codes:

"our group is using the XXX software, and recently we are going to buy a 64-bit multiprocessor server. We narrowed down our considerations to three architectures, but apart from performance we also take into considerations the availability of the software. Please, could you let me know whether XXX is running (compilable) on the following 64-bit CPUs:

UltraSPARC III  
IBM Power 4+ (IBM p650)  
Intel Itanium 2 (SGI Altrix 3000)"

## **2.1 Gamess (Mark Gordon)**

”Yes, GAMESS runs on all three. We have an UltraSPARC system in house, will have a new SGI system in April, and hopefully an IBM Power4 is on the horizon.”

## **2.2 Gaussian (Wendy G. Janocha - Sales manager)**

”According to our technical staff, we expect Gaussian 03 to be supported on the Ultra SPARC III, it should also be supported on the IBM Power 4+, but only in compatability mode. We are considering the Intel Itanium 2 (SGI Altrix 3000) using Linux, but we do not have any information as to when this version will be supported.

## **2.3 Turbomole (Uwe Huniar)**

”currently we only have a serial version for IBM Power4.

SUN has the Turbomole source code and they are just about to port 5.6 to Solaris. The parallel version for Power4 machines is not running yet, but we are in contact with IBM to solve that problem. Work on the Linux/Itanium2 version has already begun, but since that is the only really new platform for Turbomole, it surely will take some time to port to Code.

What we do have is a 64-Bit version for HP-UX (for PA-RISC and Itanium CPUs) and a version for Tru64 Unix.”

## **2.4 Molpro (Peter J. Knowles, J. Werner)**

This is the answer from Pete Knowles:

”Ultrasparc III: I am not totally sure, but it is definitely running on a Sun of some kind with reasonably recent operating system, and in 64-bit mode. If it didn't run on your machine, our contact in Sun would almost certainly be interested to work with us in fixing any problem.

Power4: we have recently got it going on this platform, and in your timescale, it will definitely be OK.

SGI Altrix: the code now runs on HP and NEC linux IA64 systems; we are in contact with a colleague on SGI who seems keen to demonstrate that it will go on their hardware also. (He is from Czech republic, so maybe he contacted us because of you?) ”

Then I sent an e-mail with the clarification request to J. Werner:

"I'd greatly appreciate your input, as I know that you were trying to compile Molpro for Itanium CPU with Linux OS (SGI machine with RedHat) on Prof. Hobza's group computer, but you didn't succeed.

What was the problem? My guess is that it was a problem with compiler, as I don't see any reason why wouldn't be your code be compilable on Linux Itanium, when it runs smoothly on HP-UX OS (am I right)? What compiler did you use, was it 64-bit gcc or Intel Compiler? And which version?

Do you know if it is possible compile Molpro on new Itanium 2 based machines from SGI (SGI Altix 3000 with Red Hat 7.2)? According to Prof. Knowles "the code now runs on HP and NEC linux IA64 systems", so I don't see any reason, why shouldn't it be compilable on SGI? But if it is compilable on HP and NEC Linux IA64 systems (i.e. Itanium 2 systems), why couldn't you run it on Itanium 1 (provided, that the problem really was a compiler)?"

I've got the answer immediately:

"I have little to add to what Prof. Knowles already told you. The program certainly runs on Sun Ultrasparc III systems. The new version, coming out these days, also runs under hp-linux and nec-linux for ia-64 using the Intel efc compiler (Redhat). Also it runs efficiently under hp-ux11.22. We have no possibility to test on sgi at present, but I can't see any reason why it should not be possible to get it working. The problems in our first attempts on Hobza's machine should now be solved. The performance will be strongly dependent on the efficiency of blas libraries provided by the vendors. There are very good ones for HP, but I don't know about the other systems. Concerning price/performance, the new HP workstations are very good; The IBM power4 systems are FAR too expensive and not worth the money (the memory bandwidth is too small). Sun Ultrasparc III is probably a factor of 2 slower (per processor)."

## 2.5 Molcas (Valera Veryazov)

"Molcas is running under Solaris on Ultra SPARC (there is a problem with some versions of compiler:

<http://www.teokem.lu.se/molcas/wwwboard/messages/320.html>), under xlf

6.1/7.1/8.1 on AIX 4.3/5.1 on Power 4. Version with Intel Itanium2 is under testing....”

## 2.6 Amber (different sources)

Amber maintainers advised me to send my questions to the Amber’s mailing list, here are the responses:

”We’ve built Amber7 + patches through number 32 on an HP ZX6000 Itanium-2 system, using the most recent version of Intel’s Fortran compiler, Version 7.0. It passes all of the tests, and runs with good speed.”

”I am using Amber7 on Compaq Alpha (Tru64 and Linux) and Itanium2 machines, and the calculation seems fastest on Itanium2 but not by a wide margin.

....

(this is a comment on the Intel Fortran Copiler 7:) The optimization level must be lowered from 3 to 2. The problem seems to arise only in a few subroutines, but it is a lot of hassle trying to work out the problem and to set the optimization levels for individual program units.”

”For Alpha, there will be no trouble on Tru64. I expect the same for Linux, assuming Compaq Fortran is used - I have done this build, though not recently. I would be very surprised if any trouble were found on OpenVMS, but I don’t speak from experience in that case.

For Itanium 2, running Linux with Intel compilers, I and others have encountered trouble (run-time errors) using -O3 optimization, but success using -O2. One option not specifically mentioned by Dr. Svozil is Itanium 2 running HP-UX. The HP compilers are 64-bit, and will build AMBER with no trouble. ”

”The IBM xlf compiler can handle 64-bit applications. Currently we build AMBER as a +32-bit application. Yes, I have built AMBER7 on the IBM p650 without any problems.”

One useful link from SGI:

”We have tested Amber7 on Altix. We supplied the machine file that builds and runs the code corectly on this machine. Look in our webpage:  
<http://www.sgi.com/industries/sciences/chembio/resources/amber/>”

## 2.7 CHARMM (Martin Karplus)

"We have little experience with those 64-bit CPU parallel computers appeared recently in the market. As surveyed among the developers, most of us have been running CHARMM parallel on (1) SGI/MPI, (2) GNU linux (Pentium, Athlon), Fast Ethernet / Myrinet / MPICH, (3) SP3/MPI. Some have used an Intel Itanium II but only in serial mode.

As for benchmarking, a note would be useful (<http://r.cmm.ki.si/vrana/amdvsintel.html>).

While the port for a given machine would not be a much problem, we do not have our hands on those machines yet." (answer by Youngdo Wona)

## 2.8 Gromos (van Gunsteren)

N/A

# 3 Comments on individual architectures

UltraSPARC is about half as fast as the others (Alpha, Power4+ and Itanium 2 are of about the same power depending on the type of the problem). Excellent benchmarks on the computational chemistry may be found here: <http://www.dl.ac.uk/CFS/benchmarks/compchem.html>.

## 3.1 IBM Power4/4+

- expensive (??? not entirely true, IMHO)  
"The IBM power4 systems are FAR too expensive and not worth the money" (J. Werner)
- disadvantage: low memory bandwidth (J. Werner, WWW sources)  
"I can tell you about molcas running rasscf, caspt2 calculations. It seems that cpu performances are comparable between these machines. However, for the I/O performances (that are really important with molcas because some large caspt2 calculations you may need 40 Gb of disk), I can really advise not to buy the power4. Moreover, buying all the disk and ram you need could be a little (!) expensive." (Nicolas Ferre, University of Siena, Italy)
- not used in CC very often  
"Power4+ systems, I would guess, are more expensive and Power4+/AIX

may have less support among quantum chemistry codes. I've just never read about anyone using this for actual quantum chem work." (Brian Barnes)

## 3.2 Alpha

- The future of Alpha is very unclear, according to different WWW sources HP will not develop Alpha any further, the latest version will be Alpha EV78 (middle of 2003??). Intel has bought some key Alpha technologies and employed some of Alpha engineers, so the Alpha features will probably appear in the future in Itanium CPUs.  
"Alpha's an orphan, and might vanish any day now." (J. Leonard)  
"the Alpha is at its end-of-line. There will be no new generations to that chip. you'll have to switch architectures in a few years anyway if you buy this." (B. Barnes)
- expensive  
"Itanium2 machines are however a lot less expensive than Alpha machines so I am in the process of migrating from Alpha to Itanium2." (Tadashi Takemori, Institute of Materials Science, University of Tsukuba, Tsukuba, Ibaraki 305-8573, Japan)
- the best OS for Alpha is Tru64  
"Alpha machines run best with Tru64 plus Compaq Fortran (Fortran compiler IS available for Linux Alpha, but slightly slower than on Tru64). The compiled binary code still runs on Linux machines so I copy the binary codes to Linux Alpha after compiling on Tru64 machines." (Tadashi Takemori, Institute of Materials Science, University of Tsukuba, Tsukuba, Ibaraki 305-8573, Japan)
- Linux models are cheaper than those with Tru64  
"Linux models are a lot cheaper than the Tru64 models." (Tadashi Takemori, Institute of Materials Science, University of Tsukuba, Tsukuba, Ibaraki 305-8573, Japan)

## 3.3 Itanium 2

- The problem of Molpro's non-compileability on Itanium 1 (SGI machine, but I guess it concerns all the Itanium 1 machines) is solved for Itanium 2.  
"The new version, coming out these days, also runs under hp-linux and nec-linux for ia-64 using the Intel ifc compiler (Redhat). Also it

runs efficiently under hp-ux11.22. We have no possibility to test on sgi at present....The problems in our first attempts on Hobza's machine should now be solved. The performance will be strongly dependent on the efficiency of blas libraries provided by the vendors. There are very good ones for HP, but I don't know about the other systems.." (J. Werner)

- The only option (apart from slow GCC) for Linux system is Intel C/C++ or Intel Fortran Compiler (actual version 7). But this compiler is not without bugs

"....still buggy Intel compiler" (Valera Verazov)

Buggy was mainly the version 5, but qthe compiler quality is improving  
"We've built Amber7 + patches through number 32 on an HP ZX6000 Itanium-2 system, using the most recent version of Intel's Fortran compiler, Version 7.0. It passes all of the tests, and runs with good speed. It does the same with GAMESS-US, so I wouldn't worry about problems with the Intel compilers at this stage. 5.1 had problems" (Frederick P. Arnold, Jr., NUIT, Northwestern U.)

"However, apparently the HP/Compaq merger has allowed Intel to hire away many of the best compiler writers who worked on Tru64 for Compaq and DEC before that. So, Intel has made a strong commitment to their compilers and you can probably expect them to improve quickly." (B. Krueger)

Do not use -O3 optimization in Intel Compiler, -O2 is fine.

"For Itanium 2, running Linux with Intel compilers, I and others have encountered trouble (run-time errors) using -O3 optimization, but success using -O2." (C. Schneider, HP)

- Here is another option for HP Itanium 2 systems (my personal remark: HP doesn't offer 8 CPUs Itanium 2 system yet, it will be released in the second half of 2003)

"One option not specifically mentioned by Dr. Svozil is Itanium 2 running HP-UX. The HP compilers are 64-bit, and will build AMBER with no trouble." (C. Schneider, HP)

- Information about GCC 64-bit compiler od SGI machine

"Do be sure (hopefully SGI will have done this already) to upgrade, or at least install, GCC 3.2.2, and its associated libraries should you go the Itanium-2 route. RedHat's 2.96 series compiler shipped with RH 7.2 Advanced Server is unreliable on the Itanium-2, as well as being slow." (Frederick P. Arnold, Jr., NUIT, Northwestern U.)

- no low-bandwidth problem with Itanium 2