

(28 Nov 2005)

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* Section 5 - Programmer's Reference *
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This section describes features of GAMESS programming which are true for all machines. See the section 'hardware specifics' for information about specific machines. The contents of this section are:

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Installation overview

Very specific compiling directions are given in a file provided with the GAMESS distribution, namely

~/gamess/misc/readme.unix

and this should be followed closely. The directions here are of a more general nature.

Before starting the installation, you should also see the pages about your computer in the 'Hardware Specifics' section of this manual, and at the compiler version notes that are kept in the script 'comp'. There might be some special instructions for your machine.

The first step in installing GAMESS should be to print the manual. If you are reading this, you've got that done! The second step would be to get the source code activator compiled and linked (note that the activator must be activated manually before it is compiled). Third, you should now compile all the quantum chemistry sources. Fourth, compile the DDI message passing library, and its process kickoff program. Fifth, link the GAMESS program. Finally, run all the short examples provided with GAMESS, and very carefully compare the key results shown in the 'sample input' section against your outputs. These "correct" results are from a IBM RS/6000, so there may be very tiny (last digit) precision differences for other machines. That's it! The rest of this section gives a little more detail about some of these steps.

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GAMESS will run on essentially any machine with a FORTRAN 77 compiler. However, even given the F77 standard there are still a number of differences between various machines. For example, some chips still use 32 bit integers, as primitive as that may seem, while many chips allow for 64 bit processing (and hence very large run-time memory usage). It is also necessary to have a C compiler, as the message passing library is implemented entirely in that language.

Although there are many types of computers, there is only one (1) version of GAMESS.

This portability is made possible mainly by keeping machine dependencies to a minimum (that is, writing in

FORTRAN77, not vendor specific language extensions). The unavoidable few statements which do depend on the hardware are commented out, for example, with "*I64" in columns 1-4. Before compiling GAMESS on a 64 bit machine, these four columns must be replaced by 4 blanks. The process of turning on a particular machine's specialized code is dubbed "activation".

A semi-portable FORTRAN 77 program to activate the desired machine dependent lines is supplied with the GAMESS package as program ACTVTE. Before compiling ACTVTE on your machine, use your text editor to activate the very few machine dependent lines in ACTVTE before compiling it. Be careful not to change the DATA initialization!

* * * * *

The quantum chemistry source code of GAMESS is in the directory

~/gamess/source

and consists almost entirely of unactivated FORTRAN source code, stored as *.src. There is a bit of C code in this directory to implement runtime memory allocation.

The task of building an executable for GAMESS is:

	activate	compile	link
*.SRC --->	*.FOR --->	*.OBJ --->	*.EXE
source	FORTTRAN	object	executable
code	code	code	image

where the intermediate files *.FOR and *.OBJ are discarded once the executable has been linked. It may seem odd at first to delete FORTRAN code, but this can always be reconstructed from the master source code using ACTVTE.

The advantage of maintaining only one master version is obvious. Whenever any improvements are made, they are automatically in place for all the currently supported machines. There is no need to make the same changes in a plethora of other versions.

* * * * *

The Distributed Data Interface (DDI) is the message passing layer, supporting the parallel execution of GAMESS. It is stored in the directory tree

~/gamess/ddi

It is necessary to compile this software, even if you don't intend to run on more than one processor. This directory contains a file readme.ddi with directions about compiling,

and customizing your computer to enable the use of System V memory allocation routines. It also has information about some high end parallel computer systems.

* * * * *

The control language needed to activate, compile, and link GAMESS on your brand of computer involves several scripts, namely:

COMP compiles a single quantum chemistry module.
COMPALL compiles all quantum chemistry source modules.
COMPDDI compiles the distributed data interface, and
 generates a process kickoff program, ddikick.x.
LKED link-edit (links) together quantum chemistry
 object code, and the DDI library, to produce a
 binary executable gamess.x.
RUNGMS runs a GAMESS job, in serial or parallel.
RUNALL uses RUNGMS to run all the example jobs.

There are files related to some utility programs:

MBLDR.* model builder (internal to Cartesian)
CARTIC.* Cartesian to internal coordinates
CLEMNO.* cleans up \$VEC groups
DK3.F prepare relativistic A0 contractions.

There are files related to two-D X windows graphics, in:

~/gamess/graphics

although if you have an Apple computer (lucky you!), you should obtain Brett Bode's MacMolPlt program, which has the same graphics capabilities, and much more.

Running Distributed Data Parallel GAMESS

GAMESS consists of many FORTRAN files implementing its quantum chemistry, and some C language files implementing the Distributed Data Interface (DDI). The directions for compiling DDI, configuring the system parameters to permit execution of DDI programs, and how to use the 'ddikick.x' program which "kicks off" GAMESS processes may be found in the file readme.ddi. If you are not the person installing the GAMESS software, you can skip reading that.

Efficient use of GAMESS requires an understanding of three critical issues: The first is the difference between two types of memory (replicated MEMORY and distributed MEMDDI) and how these relate to the physical memory of the computer which you are using. Second, you must understand to some extent the degree to which each type of computation scales so that the proper number of nodes is selected. Finally, many systems run *-two-* GAMESS processes on every processor, and if you read on you will find out why this is so.

Since all code needed to implement the Distributed Data Interface (DDI) is provided with the GAMESS source code distribution, the program compiles and links ready for parallel execution on all machine types. Of course, you may choose to run on only one processor, in which case GAMESS will behave as if it is a sequential code, and the full functionality of the program is available.

parallelization history

We began to parallelize GAMESS in 1991 as part of the joint ARPA/Air Force piece of the Touchstone Delta project. Today, nearly all ab initio methods run in parallel, although some of these still have a step or two running sequentially only. Only the RHF+CI gradients have no parallel method coded. We have not parallelized the semi-empirical MOPAC runs, and probably never will. Additional parallel work occurred as a result of a DoD CHSSI software initiative in 1996. This led to the DDI-based parallel RHF+MP2 gradient program, after development of the DDI programming toolkit itself. Since 2002, the DoE program SciDAC has sponsored additional parallelization. The DDI toolkit has been used since its 1999 introduction to add codes for UHF+MP2 gradient, ROHF+ZAPT2 energy, and MCSCF

wavefunctions as well as their analytic Hessians or MCQDPT2 energy correction.

In 1991, the parallel machine of choice was the Intel Hypercube although small clusters of workstations could also be used as a parallel computer. In order to have the best blend of portability and functionality, we chose in 1991 to use the TCGMSG message passing library rather than one of the early vendor's specialized libraries. As the major companies began to market parallel machines, and as MPI version 1 emerged as a standard, we began to use MPI on some equipment in 1996, while still using the very resilient TCGMSG library on everything else. However, in June 1999, we retired our old friend TCGMSG when the message passing library used by GAMESS changed to the Distributed Data Interface, or DDI. An SMP-optimized version of DDI was included with GAMESS in April 2004.

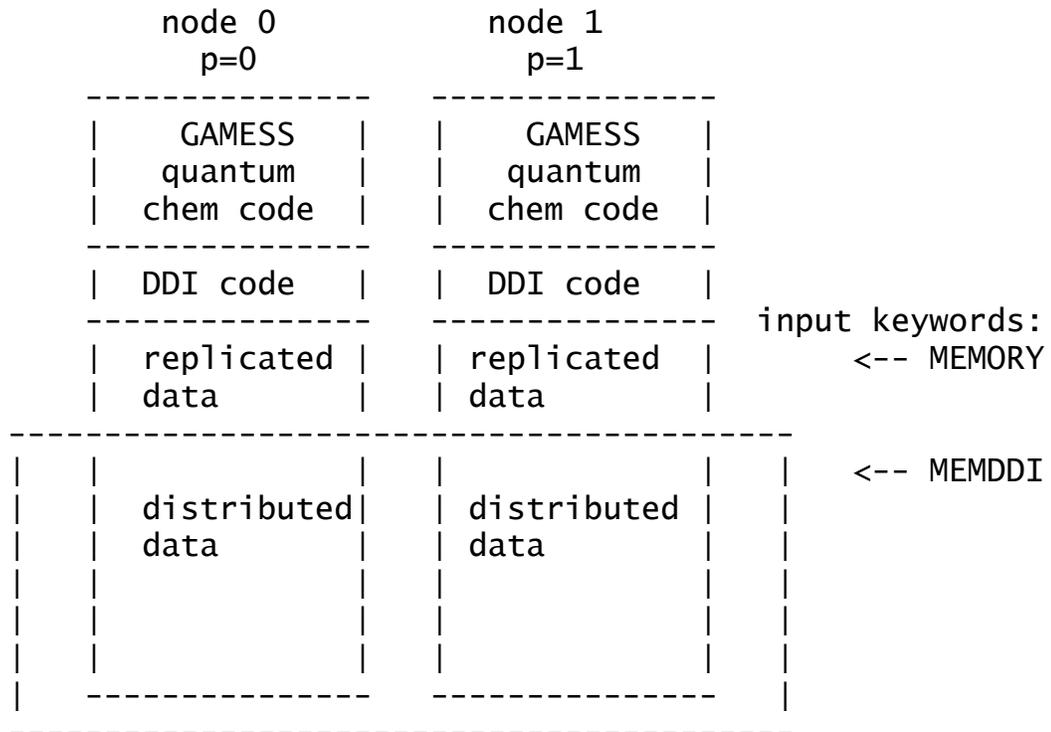
Three people have been extremely influential upon the current parallel methodology. Theresa Windus, a graduate student in the early 1990s, created the first parallel versions. Graham Fletcher, a postdoc in the late 1990s, is responsible for the addition of distributed data programming concepts. Ryan Olson rewrote the DDI software in 2003-4 to support the modern SMP architectures well, and this was released in April 2004 as our standard message passing implementation.

DDI compute and data server processes

DDI contains the usual parallel programming calls, such as initialization/closure, point to point messages, and the collective operations global sum and broadcast. These simple parts of DDI support all parallel methods developed in GAMESS from 1991-1999, which were based on replicated storage rather than distributed data. However, DDI also contains additional routines to support distributed memory usage.

DDI attempts to exploit the entire system in a scalable way. While our early work concentrated on exploiting the use of p processors and p disks, it required that all data in memory be replicated on every one of the p nodes. The use of memory also becomes scalable only if the data is distributed across the aggregate memory of the parallel machine. The concept of distributed memory is contained in the Remote Memory Access portion of MPI version 2, but so far MPI-2 is not available from American computer vendors.

The Cray T3E has a library named SHMEM to support this type of one sided messages (and good hardware support for this too) so, on the T3E, GAMESS runs as a single process per CPU. Its memory image looks like this:



where the box drawn around the distributed data is meant to imply that a large data array is residing in the memory of all nodes (in this example, half on one and half on the other).

Note that the input keyword MEMORY gives the amount of storage used to duplicate small matrices on every node, while MEMDDI gives the -total- distributed memory required by the job. Thus, if you are running on p nodes, the memory that is used on any given node is

$$\text{total on any 1 node} = \text{MEMORY} + \text{MEMDDI}/p$$

Since MEMDDI is very large, its units are in millions of words. The keyword MEMORY is in units of words (64 bit quantity) and so you must either convert units carefully or use the MWORDS synonym for MEMORY (for which the units are also millions of words). Since good execution speed requires that you not exceed the physical memory belonging to your nodes, it is important to understand that when MEMDDI is large, you will need to choose a sufficiently large number of nodes to keep the memory on each node

reasonable.

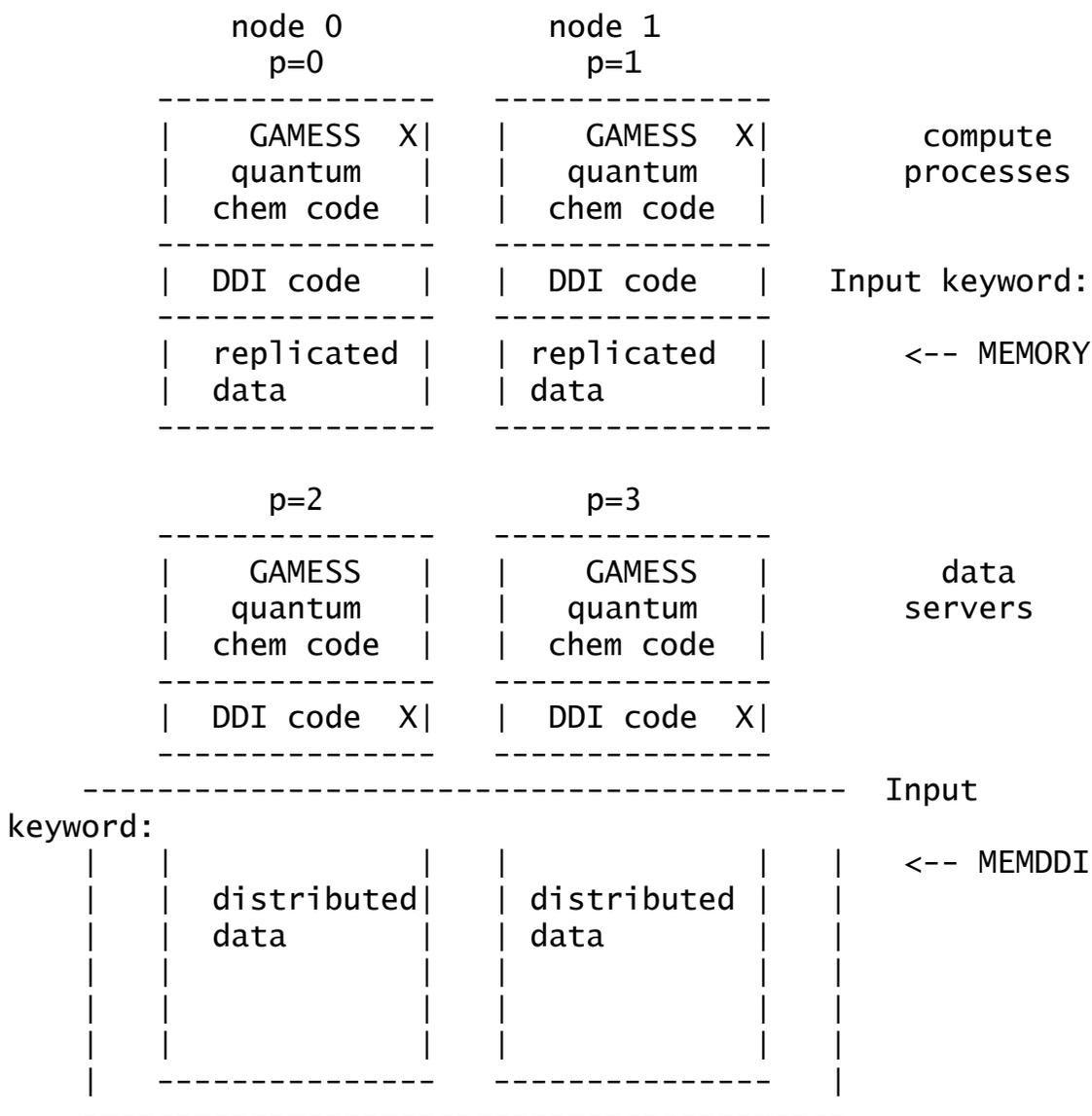
To repeat, the DDI philosophy is to add more processors not just for their compute performance or extra disk space, but also to aggregate a very large total memory. Bigger problems will require more nodes to obtain sufficiently large total memories! We will give an example of how you can estimate the number of nodes a little ways below.

If the GAMESS task running as process $p=1$ in the above example needs some values previously computed, it issues a call to `DDI_GET`. The DDI routines in process $p=1$ then figure out where this "patch" of data actually resides in the big rectangular distributed storage. Suppose this is on process $p=0$. The DDI routines in $p=1$ send a message to $p=0$ to interrupt its computations, after which $p=0$ sends a bulk data message to process $p=1$'s buffer. This buffer resides in part of the replicated storage of $p=1$, where computations can occur. Note that the quantum chemistry layer of process $p=1$ was sheltered from most of the details regarding which node owned the patch of data that process $p=1$ wanted to obtain. These details are managed by the DDI layer.

Note that with the exception of `DDI_ACC`'s addition of new terms into a distributed array, no arithmetic is done directly upon the distributed data. Instead, distributed data is accessed only by `DDI_GET`, `DDI_PUT` (its counterpart for storage of data items), and `DDI_ACC` (which accumulates new terms into the distributed data). `DDI_GET` and `DDI_PUT` can be thought of as analogous to FORTRAN `READ` and `WRITE` statements that transfer data between disk storage and local memory where computations may occur.

It is the programmer's challenge to minimize the number of `GET/PUT/ACC` calls, and to design algorithms that maximize the chance that the patches of data are actually within the local node's portion of the distributed data.

Since the SHMEM library is available only on a few machines, all other platforms adopt the following memory model, which involves -two- GAMESS processes running on every processor:



The first half of the processes do quantum chemistry, and the X indicates that they spend most of their time executing some sort of chemistry. Hence the name "compute process". Soon after execution, the second half of the processes call a DDI service routine which consists of an infinite loop to deal with GET, PUT, and ACC requests until such time as the job ends. The X shows that these "data servers" execute only DDI support code. (This makes the data server's quantum chemistry routines the equivalent of the human appendix). The whole problem of interrupts is now in the hands of the operating system, as the data servers

are distinct processes. To follow the same example as before, when the compute process $p=1$ needs data that turns out to reside on node 0, a request is sent to the data server $p=2$ to transfer information back to the compute process $p=1$. The compute process $p=0$ is completely unaware that such a transaction has occurred.

The formula for the memory required by any single node is unchanged, if p is the total number of nodes used,
total on any 1 node = MEMORY + MEMDDI/ p .

As a technical matter, if you are running on a system where all processors are in the same node (the SGI Altix is an example), or if you are running on an IBM SP where LAPI assists in implementing one-sided messaging, then the data server processes are not started. The memory model in the illustration above is correct, if you just mentally omit the data server processes from it. In all cases, where the SHMEM library is not used, the distributed arrays are created by System V memory calls, shmget/shmat, and their associated semaphore routines. Your system may need to be reconfigured to allow allocation of large shared memory segments, see 'readme.ddi' for more details.

memory allocations and check jobs

At present, not all runs require distributed memory. For example, in an SCF computation (no hessian or MP2 to follow) the memory needed is on the order of the square of the basis set size, for such quantities as the orbital coefficients, density, Fock, overlap matrices, and so on. These are simply duplicated on every node in the MEMORY region. In this case the data server processes still run, but are dormant because no distributed memory access is attempted.

However, closed and open shell MP2 calculations, MCSCF wavefunctions, and their analytic hessian or MCQPDT energy correction do use distributed memory when run in parallel. Thus it is important to know how to obtain the correct value for MEMDDI in a check run.

Check runs (EXETYP=CHECK) need to run quickly, and the fastest turn around always comes on one node only. Runs which do not currently exploit MEMDDI distributed storage will formally allocate their MEMORY needs, and feel out their storage needs while skipping almost all of the real work. Since MEMORY is replicated, the amount that is

needed on 1 node remains unchanged if you later do the true computation on more than 1 node.

Check jobs which involve MEMDDI storage are a little bit trickier. As noted, we want to run on only 1 node to get fast turn around. However, MEMDDI is typically a large amount of memory, and this is unlikely to be available on a single node. The solution is that the data server process does not actually allocate the MEMDDI storage, instead it just remembers what you gave as input and checks to see if this will be adequate. So, you can input MEMDDI=1000 (1000 million words is equal to $1,000 * 1,000,000 * 8 = 8$ GBytes and run this check job on a computer with only 256 MB of RAM.

Of course, the actual computation will have to run on a large number of such processors. Let us continue with this example of a run requiring 8 GBytes of distributed data on 256 MB nodes. Suppose that MEMORY is 2500000 in this case (when MEMDDI is used, MEMORY is typically just a few million words). We need to reserve some memory for the operating system (16 MBytes, say) and for the GAMESS program and local storage (approx 16 MB, it is a big program, and the compute processes should be swapped into memory). Thus our hypothetical 256 MB node has 224 MB available, assuming no one else is running. The rest of the computations proceed in million/mega words, so the available memory per node is $224/8 = 28$. We must choose the number of processors p to satisfy

needed \leq available

MEMORY + MEMDDI/ p \leq free physical memory

$2.5 + 1000/p \leq 28$

so this example requires $p \geq 39$ compute processes.

One more subtle point about CHECK runs with MEMDDI is that since you are running on 1 node only, the code does not know that you wish to run the parallel algorithm instead of the sequential algorithm. You must force the CHECK job into the parallel section of the program by

\$system parall=.true. \$end

There's no harm leaving this line in for the true runs, as any job with more than one compute process is parallel regardless of the input value PARALL.

The check run for MCQDPT jobs will print three times a line like this

MAXIMUM MEMDDI THAT CAN BE USED IN ... IS x MWORDS

Typically the 2nd such step, transforming over all occupied and virtual canonical orbitals, will be the

largest of the three requirements. Its size can be guesstimated before running, as

$$(Nao*Nao+Nao)/2 * ((Nocc*Nocc+Nocc)/2 + Nocc*Nvirt)$$

where $Nocc = NMOFZC + NMODOC + NMOACT$, $Nvirt = NMOEXT$, and Nao is the size of the atomic basis. Unlike the closed shell MP2 program, this section still does extensive I/O operations even when MEMDDI is used, so it may be useful to consider the three input keywords DOORD0, PARAI0, and DELSCR when running this code.

representative performance examples

This section describes the way in which the various quantum chemistry computations run in parallel, and shows some typical performance data. This should give you as the user some idea how many nodes can be efficiently used for various SCFTYP and RUNTYP jobs

The performance data you will see below were obtained on a 16 node Intel Pentium II Linux (Beowulf-type) cluster costing \$49,000, of which \$3,000 went into the switched Fast Ethernet component. 512 MB/node means this cluster has an aggregate memory of 8 GB. For more details, see <http://www.msg.ameslab.gov/GAMESS/dist.pc.shtml>. This is a low quality network, which exposes jobs with higher communication requirements, by noting when the wall time is much longer than the CPU.

The HF wavefunctions can be evaluated in parallel using either conventional disk storage of the integrals, or via direct recomputation of the integrals. Some experimenting will show which is more effective on your hardware. As an example of the scaling performance of RHF, ROHF, UHF, or GVB jobs that involve only computation of the energy or its gradient, we include here a timing table from the 16 node PC cluster. The molecule is luciferin, which together with the enzyme luciferase is involved in firefly light production. The chemical formula is C₁₁N₂S₂O₃H₈, and RHF/6-31G(d) has 294 atomic orbitals. There's no molecular symmetry. The run is done as direct SCF, and the CPU timing data is

	p=1	p=2	p=4	p=8	p=16
1e- ints	1.1	0.6	0.4	0.3	0.2
Huckel guess	14	12	11	10	10

15 RHF iters	5995	2982	1493	772	407	
properties	6.0	6.6	6.6	6.8	6.9	
1e- gradient	9.7	4.7	2.3	1.2	0.7	
2e- gradient	1080	541	267	134	68	
	----	----	----	----	----	
total CPU	7106	3547	1780	925	492	seconds
total wall	7107	3562	1815	950	522	seconds

Note that direct SCF should run with the wall time very close to the CPU time as there is essentially no I/O and not that much communication (MEMDDI storage is not used by this kind of run). Running the same molecule as DFTTYP=B3LYP yields

	p=1	p=2	p=4	p=8	p=16
1e- ints	1.1	0.7	0.3	0.3	0.2
Huckel guess	14	12	10	10	9
23 DFT iters	14978	7441	3681	1876	961
properties	6.6	6.4	6.5	7.0	6.5
1e- gradient	9.7	4.7	2.3	1.3	0.7
2e- grid grad	5232	2532	1225	595	303
2e- AO grad	1105	550	270	136	69
	----	----	----	----	----
total CPU	21347	10547	5197	2626	1349
total wall	21348	10698	5368	2758	1477

and finally if we run an RHF analytic hessian, using A0 basis integrals, the result is

	p=1	p=2	p=4	p=8	p=16
1e- ints	1.2	0.6	0.4	0.3	0.2
Huckel guess	14	12	10	10	10
14 RHF iters	5639	2851	1419	742	390
properties	6.4	6.5	6.6	7.0	6.7
1e- grd+hss	40.9	20.9	11.9	7.7	5.8
2e- grd+hss	21933	10859	5296	2606	1358
CPHF	40433	20396	10016	5185	2749
	-----	-----	-----	-----	-----
total CPU	68059	34146	16760	8559	4519
total wall	68102	34273	17430	9059	4978

CPU speedups for 1->16 processors for RHF gradient, DFT gradient, and RHF analytic hessian are 14.4, 15.8, and 15.1 times faster, respectively. The wall clock times are close to the CPU time, indicating very little communication is involved. If you are interested in an explanation of how the parallel SCF is implemented, see the main GAMESS paper, M.W.Schmidt, K.K.Baldrige, J.A.Boatz, S.T.Elbert, M.S.Gordon, J.H.Jensen, S.Koseki, N.Matsunaga,

K.A.Nguyen, S.J.Su, T.L.Windus, M.Dupuis, J.A.Montgomery
 J.Comput.Chem. 14, 1347-1363(1993)

The CIS energy and gradient code is also programmed to have the construction of Fock-like matrices as its computational kernel. Its scaling is therefore very similar to that just shown, for porphin C₂₀N₄H₁₄, DH(d,p) basis, 430 AOs:

	p=1	p=2	p=4	p=8	p=16
setup	25	25	25	25	25
1e- ints	5.1	2.7	1.5	1.0	0.6
orb. guess	30	25	23	22	21
RHF iters	1647	850	452	251	152
RHF props	19	19	19	19	19
CIS energy	36320	18166	9098	4620	2398
CIS lagrang	6092	3094	1545	786	408
CPHF	20099	10183	5163	2688	1444
CIS density	2468	1261	632	324	170
CIS props	19	19	19	19	19
1e- grad	40.9	18.2	9.2	4.7	2.4
2e- grad	1644	849	423	223	122
	-----	-----	-----	-----	-----
total CPU	68424	34526	17420	8994	4791
total wall	68443	34606	17853	9258	4985

which is a speedup of 14.3 for 1->16.

For the next type of computation, we discuss the MP2 correction. For closed shell RHF + MP2 and unrestricted UHF + MP2, the gradient program runs in parallel using distributed memory, MEMDDI. In addition, the ROHF + MP2 energy correction for OSPT=ZAPT runs in parallel using distributed memory, but OSPT=RMP does not use MEMDDI in parallel jobs. All distributed memory parallel MP2 runs resemble RHF+MP2, which is therefore the only example given here.

The example is a benzoquinone precursor to hongconin, a cardioprotective natural product. The formula is C₁₁₀H₁₀, and 6-31G(d) has 245 AOs. There are 39 valence orbitals included in the MP2 treatment, and 15 core orbitals. MEMDDI must be 156 million words, so the memory computation that was used above tells us that our 512 MB/node PC cluster must have at least three processors to aggregate the required MEMDDI. MOREAD was used to provide converged RHF orbitals, so only 3 RHF iterations are performed. The

timing data are CPU and wall times (seconds) in the 1st/2nd lines:

	p=3	p=4	p=12	p=16
RHF iters	241	181	65	51
	243	184	69	55
MP2 step	5,953	4,399	1,438	1,098
	7,366	5,669	2,239	1,700
2e- grad	1,429	1,135	375	280
	1,492	1,183	413	305
	-----	-----	---	---
total CPU	7,637	5,727	1,890	1,440
total wall	9,116	7,053	2,658	2,077
		3-->12	4-->16	
CPU speedup		4.04	3.98	
wall speedup		3.43	3.40	

The wall clock time will be closer to the CPU time if the quality of the network between the computer is improved (remember, this run used just switched Fast Ethernet). As noted, the number of nodes is more influenced by a need to aggregate the necessary total MEMDDI, more than by concerns about scalability. MEMDDI is typically large for MP2 parallel runs, as it is proportional to the number of occupied orbitals squared times the number of AOs squared.

For more details on the distributed data parallel MP2 program, see

- G.D.Fletcher, A.P.Rendell, P.Sherwood
Mol.Phys. 91, 431-438(1997)
- G.D.Fletcher, M.W.Schmidt, M.S.Gordon
Adv.Chem.Phys. 110, 267-294 (1999)
- G.D.Fletcher, M.W.Schmidt, B.M.Bode, M.S.Gordon
Comput.Phys.Commun. 128, 190-200 (2000)

The next type of computation we will consider is analytic computation of the nuclear Hessian (force constant matrix). The performance of the RHF program, based on AO integrals, was given above, as its computational kernel (Fock-like builds) scales just as the SCF itself. However, for high spin ROHF, low spin open shell SCF and TCSCF (both done with GVB), the only option is MO basis integrals. The integral transformation is parallel according to

- T.L.Windus, M.W.Schmidt, M.S.Gordon
Theoret.Chim.Acta 89, 77-88(1994).

It distributes 'passes' over nodes, so as to parallelize the transformation's CPU time but not the replicated memory, or the AO integral time. Finally the response equation step is hardly parallel at all. The test example is an intermediate in the ring opening of silacyclobutane, GVB-PP(1) or TCSCF, 180 AOs for 6-311G(2d,2p):

	p=1	p=2	p=4	p=8	p=16
2e- ints	83	42	21	11	5
GVB iters	648	333	179	104	67
replicate 2e-	n/a	81	81	81	82
transf.	476	254	123	67	51
1e- grd+hss	7	4	2	2	1
2e- grd+hss	4695	2295	1165	596	313
CP-TCSCF	344	339	331	312	325
	----	----	----	----	----
total CPU	6256	3351	1904	1189	848
total wall	6532	3538	2072	1399	1108

Clearly, the final response equation (CPHF) step is a sequential bottleneck, as is the fact that the orbital hessian in this step is stored entirely on the disk space of node 0. Since the integral transformation is run in replicated MEMORY rather than distributing this, and since it also needs a duplicated AO integral file be stored on every node, the code is clearly not scalable to very many processors. Typically we would not request more than 3 or 4 processors for an analytic ROHF or GVB hessian.

The final analytic hessian type is for MCSCF. The scalability of the MCSCF wavefunction will be given just below, but the response equation step for MCSCF is clearly quite scalable. The integral transformation for the response equation step uses distributed memory MEMDDI, and should scale like the MP2 program (documented above). The test case has 8e- in 8 orbitals, and the time reflect this, with most of the work involving the 4900 determinants. Total speedup for 4->16 is 4.11, due to luckier work distributing for 16 CPUs:

	p=4	p=16	
MCSCF wfn	113.5	106.1	
DDI transf.	68.4	19.3	
1e- grd+hss	1.5	0.6	
2e- grd+hss	2024.9	509.8	
CPMCHF RHS	878.8	225.8	(RHS=right hand
sides)			
CPMCHF iters	115343.5	27885.9	
	-----	-----	
total CPU	118430.8	28747.6	

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total wall      119766.0   30746.4
```

This code can clearly benefit from using many processors, with scalability of the MCSCF step itself almost moot.

Now lets turn to MCSCF energy/gradient runs. We will illustrate two convergers, SOSCF and then FULLNR. The former uses a 'pass' type of integral transformation (ala the GVB hessian job above), and runs in replicated memory only (no MEMDDI). The FULLNR converger is based on the MP2 program's distributed memory integral transformation, so it uses MEMDDI. In addition, the parallel implementation of the FULLNR step never forms the orbital hessian explicitly, doing Davidson style iterations to predict the new orbitals. Thus the memory demand is almost entirely MEMDDI.

The example we choose is at a transition state for the water molecule assisted proton transfer in the first excited stat of 7-azaindole. The formula is C7N2H6(H2O), there are 190 active orbitals, and the active space is the 10 pi electrons in 9 pi orbitals of the azaindole portion. There are 15,876 determinants used in the MCSCF calculation, and 5,292 CSFs in the perturbation calculation to follow. See Figure 6 of G.M.Chaban, M.S.Gordon J.Phys.Chem.A 103, 185-189(1999) if you are interested in this chemistry. The timing data for the SOSCF converger are

	p=1	p=2	p=4	p=8	p=16
dup. 2e- ints	327.6	331.3	326.4	325.8	326.5
transform.	285.1	153.6	88.4	57.8	47.3
det CI	39.3	39.4	38.9	38.3	38.1
2e- dens.	0.4	0.5	0.5	0.5	0.5
orb. update	39.2	25.9	17.4	12.8	11.0
iters 2-16	5340.0	3153.5	2043.7	1513.6	1308.5
1e- grad	5.3	2.3	1.3	0.7	0.4
2e- grad	695.6	354.9	179.4	93.2	50.9
	-----	-----	-----	-----	-----
total CPU	6,743	4,071	2,705	2,052	1,793
total wall	13,761	8,289	4,986	3,429	3,899

whereas the FULLNR convergers runs like this

	p=1	p=2	p=4	p=8	p=16
2e- DDI trans.	2547	1385	698	354	173
det. CI	39	39	38	38	38

DM2	0.5	0.5	0.5	0.5	0.5
FULLNR	660	376	194	101	51
iters 2-9	24324	13440	6942	3669	1940
1e- grad	5.3	2.3	1.2	0.7	0.4
2e- grad	700	352	181	95	51
	-----	-----	-----	-----	-----
total CPU	28,288	15,605	8,066	4,268	2,265
total wall	28,290	20,719	12,866	8,292	5,583

The first iteration is broken down into its primary steps from the integral transformation to the orbital update, inclusive. The SOSCF program is clearly faster, and should be used when the number of processors is modest (say up to 8), however the largest molecules will benefit from using more processors and the much more scalable FULLNR program.

One should note that the CI calculation was done by CISTEP=ALDET, which is not presently scalable at all. This doesn't matter for small active spaces like 10 e- in 9 orbitals, as you can see above, but this program's use of replicated memory and large CPU time for big active spaces limits MCSCF scalability in the large active space limit.

Now let's consider the second order perturbation correction for this example. As noted, it is an excited state, so the test corrects two states simultaneously (S0 and S1). The parallel multireference perturbation program is described in

H.Umeda, S.Koseki, U.Nagashima, M.W.Schmidt
J.Comput.Chem. 22, 1243-1251 (2001)

The run is given the converged S1 orbitals, so that it can skip directly to the perturbation calculation:

	p=1	p=2	p=4	p=8	p=16
2e- ints	332	332	329	328	331
MCQDPT	87921	43864	22008	11082	5697
	-----	-----	-----	-----	-----
total CPU	88261	44205	22345	11418	6028
total wall	91508	45818	23556	12350	6852

This corresponds to a speedup for 1->16 of 14.6.

In summary, most ab initio computations will run in less time on more than one node. However, some things can be run only on 1 node, namely

- semi-empirical runs
- RHF+CI gradient
- Coupled-Cluster calculations

Some steps run with little or no speedup, forming sequential bottlenecks that limit scalability. They do not prevent jobs from running in parallel, but restrict the total number of nodes that can be effectively used:

ROHF/GVB hessians: solution of response equations
 MCSCF: Hamiltonian and 2e- density matrix (CI)
 energy localizations: the orbital localization step
 transition moments/spin-orbit: the final property step
 MCQDPT reference weight option

Future versions of GAMESS will address these bottlenecks.

A short summary of the useful number of nodes (based on data like the above) would be

RHF, ROHF, UHF, GVB energy/gradient, their DFT analogs, and CIS excited states	16-32+
MCSCF energy/gradient	
SOSCF	4-8
FULLNR	8-32+
analytic hessians	
RHF	16-32+
ROHF/GVB	4-8
MCSCF	64-128+
MPLEVL=2	
RHF, UHF, ROHF OSPT=ZAPT	8-256+
ROHF OSPT=RMP energy	8
MCSCF	16+

Altering program limits

Almost all arrays in GAMESS are allocated dynamically, but some variables must be held in common as their use is ubiquitous. An example would be the common block /NSHEL/ which holds the ab initio atom's basis set. The following Unix script, which we call 'mung', changes the PARAMETER statements that set various limitations:

```
#!/bin/csh
#
#       automatically change GAMESS' built-in dimensions
#
chdir /u1/mike/games/Source
#
foreach FILE (*.src)
  set FILE=$FILE:r
  echo ===== redimensioning in $FILE =====
  echo "C dd-mmm-yy - SELECT NEW DIMENSIONS" \
    > $FILE.munged
  sed -e "/MXATM=2000/s//MXATM=500/" \
    -e "/MXAO=8192/s//MXAO=2047/" \
    -e "/MXGSH=30/s//MXGSH=30/" \
    -e "/MXSH=5000/s//MXSH=1000/" \
    -e "/MXGTOT=20000/s//MXGTOT=5000/" \
    -e "/MXRT=100/s//MXRT=100/" \
    -e "/MXFRG=1050/s//MXFRG=65/" \
    -e "/MXDFG=5/s//MXDFG=1/" \
    -e "/MXPT=2000/s//MXPT=100/" \
    -e "/MXFGPT=12000/s//MXFGPT=2000/" \
    -e "/MXSP=500/s//MXSP=100/" \
    -e "/MXTS=20000/s//MXTS=2500/" \
    $FILE.src >> $FILE.munged
  mv $FILE.munged $FILE.src
end
exit
```

The script shows how to reduce memory, by decreasing the number of atoms, and reducing storage for the effective fragment and PCM solvent models. The parameters currently used for GAMESS imply about 75 MBytes of storage tied up in common blocks, which is not unreasonable, even in a laptop. Of course, the 'mung' script can also be used to increase the dimensions!

In this script,
 MXATM = max number of ab initio atoms

MXAO = max number of basis functions
MXGSH = max number of Gaussians per shell
MXSH = max number of symmetry unique shells
MXGTOT= max number of symmetry unique Gaussians

MXRT = max number of MCSCF/CI states

MXFRG = max number of effective fragment potentials
MXDFG = max number of different effective fragments
MXPT = max number of points in any one term of any EFP
MXFGPT= maximum storage for all EFPs, and is sized for
a large number of EFPs with a small number of
points (solvent applications), or a smaller
number of EFPs with many points (biochemistry).

MXSP = max number of spheres (sfera) in PCM
MXTS = max number of tesseræ in PCM

Names of source code modules

The source code for GAMESS is divided into a number of sections, called modules, each of which does related things, and is a handy size to edit. The following is a list of the different modules, what they do, and notes on their machine dependencies.

module	description	machine dependency
-----	-----	-----
ALDECI	Ames Lab determinant full CI code	1
ALGNCI	Ames Lab determinant general CI code	
BASCCN	Dunning cc-pVxZ basis sets	
BASECP	SBKJC and HW valence basis sets	
BASEXT	DH, MC, 6-311G extended basis sets	
BASHUZ	Huzinaga MINI/MIDI basis sets to Xe	
BASHZ2	Huzinaga MINI/MIDI basis sets Cs-Rn	
BASN21	N-21G basis sets	
BASN31	N-31G basis sets	
BASPCN	Jensen polarization consistent basis sets	
BASSTO	STO-NG basis sets	
BLAS	level 1 basic linear algebra subprograms	
CCAUX	auxiliary routines for CC calculations	
CCQAUX	auxiliaries for CCSD(TQ) program	
CCQUAD	renormalized CCSD(TQ) corrections	
CCSDT	renormalized CCSD(T) program	1
CHGPEN	screening for charge penetration of EFPs	
CISGRD	CI singles and its gradient	1
COSMO	conductor-like screening model	
CPHF	coupled perturbed Hartree-Fock	1
CPMCHF	multiconfigurational CPHF	1
CPROHF	open shell/TCSCF CPHF	1
DDILIB	message passing library interface code	
DELOCL	delocalized coordinates	
DEMRPT	determinant-based MCQDPT	
DFT	grid-free DFT drivers	1
DFTAUX	grid-free DFT auxiliary basis integrals	
DFTExc	grid DFT functionals	
DFTFUN	grid-free DFT functionals	
DFTGRD	grid DFT implementation	
DFTINT	grid-free DFT integrals	1
DGEEV	general matrix eigenvalue problem	
DGESVD	single value decomposition	
DMULTI	Amos' distributed multipole analysis	
DRC	dynamic reaction coordinate	
ECP	pseudopotential integrals	

ECPDER	pseudopotential derivative integrals	
ECPLIB	initialization code for ECP	
ECPPOT	HW and SBKJC internally stored potentials	
EFCHTR	fragment charge transfer	
EFDRVR	fragment only calculation drivers	
EFELEC	fragment-fragment interactions	
EFGRD2	2e- integrals for EFP numerical hessian	
EFGRDA	ab initio/fragment gradient integrals	
EFGRDB	" " " " "	
EFGRDC	" " " " "	
EFINP	effective fragment potential input	
EFINTA	ab initio/fragment integrals	
EFINTB	" " " "	
EFPAUL	effective fragment Pauli repulsion	
EFPCM	EFP/PCM interfacing	
EFPCOV	EFP style QM/MM boundary code	
EIGEN	Givens-Householder, Jacobi diagonalization	
EOMCC	equation of motion excited state CCSD	
FFIELD	finite field polarizabilitie	
FMO	n-mer drivers for Fragment Molecular Orbital	
FMOGRD	gradient routines for FMO	
FMOINT	integrals for FMO	
FMOIO	input/output and printing for FMO	
FMOLIB	utilities for FMO	
FMOPRP	properties for FMO	
FRFMT	free format input scanner	
FSODCI	determinant based second order CI	
GAMESS	main program, single point energy and energy gradient drivers, misc.	
GLOBOP	Monte Carlo fragment global optimizer	
GRADEX	traces gradient extremals	
GRD1	one electron gradient integrals	
GRD2A	two electron gradient integrals	1
GRD2B	specialized sp gradient integrals	
GRD2C	general spdfg gradient integrals	
GUESS	initial orbital guess	
GUGDGA	Davidson CI diagonalization	1
GUGDGB	" " "	1
GUGDM	1 particle density matrix	
GUGDM2	2 particle density matrix	1
GUGDRT	distinct row table generation	
GUGEM	GUGA method energy matrix formation	1
GUGSRT	sort transformed integrals	1
GVB	generalized valence bond HF-SCF	1
HESS	hessian computation drivers	
HSS1A	one electron hessian integrals	
HSS1B	" " " "	
HSS2A	two electron hessian integrals	1
HSS2B	" " " "	

INPUTA	read geometry, basis, symmetry, etc.	
INPUTB	" " " "	
INPUTC	" " " "	
INT1	one electron integrals	
INT2A	two electron integrals (Rys)	1
INT2B	two electron integrals (s,p,L rot.axis)	
INT2C	ERIC TEI code, and its s,p routines	
INT2D	ERIC special code for d TEI	
INT2F	ERIC special code for f TEI	
INT2G	ERIC special code for g TEI	
INT2R	s,p,d,L rotated axis integral package	
INT2S	s,p,d,L quadrature code	
INT2T	s,p,d,L quadrature code	
INT2U	s,p,d,L quadrature code	
INT2V	s,p,d,L quadrature code	
INT2W	s,p,d,L quadrature code	
INT2X	s,p,d,L quadrature code	
IOLIB	input/output routines,etc.	2
LAGRAN	CI Lagrangian matrix	1
LOCAL	various localization methods	1
LOCCD	LCD SCF localization analysis	
LOCPOL	LCD SCF polarizability analysis	
MCCAS	FOCAS/SOSCF MCSCF calculation	1
MCJAC	JACOBI MCSCF calculation	
MCPINP	model core potential input	
MCPINT	model core potential integrals	
MCPL10	model core potential library	
MCPL20	" " " "	
MCPL30	" " " "	
MCPL40	" " " "	
MCPL50	" " " "	
MCPL60	" " " "	
MCPL70	" " " "	
MCPL80	" " " "	
MCQDPT	multireference perturbation theory	1
MCQDWT	weights for MR-perturbation theory	
MCQUD	QUAD MCSCF calculation	1
MCSCF	FULLNR MCSCF calculation	1
MCTWO	two electron terms for FULLNR MCSCF	1
MDEFP	molecular dynamics using EFP particles	
MM23	MMCC(2,3) corrections to EOMCCSD	
MOROKM	Morokuma energy decomposition	1
MP2	2nd order Moller-Plesset	1
MP2DDI	distributed data parallel MP2	
MP2GRD	CPHF and density for MP2 gradients	1
MPCDAT	MOPAC parameterization	
MPCGRD	MOPAC gradient	
MPCINT	MOPAC integrals	
MPCMOL	MOPAC molecule setup	

MPCMSC	miscellaneous MOPAC routines	
MTHLIB	printout, matrix math utilities	
NAMEIO	namelist I/O simulator	
NEOSTB	place holder routines	
NMR	nuclear magnetic resonance shifts	
ORDINT	sort atomic integrals	1
ORMAS1	occ. restricted multiple act. space CI	
PARLEY	communicate to other programs	
PCM	Polarizable Continuum Model setup	
PCMCAV	PCM cavity creation	
PCMCV2	PCM cavity for gradients	
PCMDER	PCM gradients	
PCMDIS	PCM dispersion energy	
PCMIEF	PCM integral equation formalism	
PCMPOL	PCM polarizabilities	
PCMVCH	PCM repulsion and escaped charge	
PRPEL	electrostatic properties	
PRPLIB	miscellaneous properties	
PRPPOP	population properties	
QEIGEN	128 bit precision RI for relativity	11
QFMM	quantum fast multipole method	
QMFM	additional QFMM code	
QMMM	temporary dummy routines	
QREL	relativistic transformations	
RAMAN	Raman intensity	
RHFUHF	RHF, UHF, and ROHF HF-SCF	1
RXNCRD	intrinsic reaction coordinate	
RYSPOL	roots for Rys polynomials	
SCFLIB	HF-SCF utility routines, DIIS code	
SCFMI	molecular interaction SCF code	
SCRIF	self consistent reaction field	
SOBRT	full Breit-Pauli spin-orbit compling	
SOFFAC	spin-orbit matrix element form factors	
SOZEFF	1e- spin-orbit coupling terms	
STATPT	geometry and transition state finder	
SURF	PES scanning	
SVPCHG	surface volume polarization (SS(V)PE)	
SVPINP	input/output routines for SS(V)PE	
SVPLEB	Lebedev grids for SS(V)PE integration	
SYMORB	orbital symmetry assignment	
SYMSLC	" " "	
TDHF	time-dependent Hartree-Fock NLO	1
TDX	extended time-dependent RHF	
TDXIO	input/output for extended TDHF	
TDXITR	iterative procedures in extended TDHF	
TDXNI	non-iterative tasks in extended TDHF	
TDXPRP	properties from extended TDHF	
TRANS	partial integral transformation	1
TRFDM2	two particle density backtransform	1

TRNSTN	CI transition moments	
TRUDGE	nongradient optimization	
UMPDDI	distributed data parallel MP2	
UNPORT	unportable, nasty code	3,4,5,6,7,8
VBDUM	dummy substitute for VB2000 program	
VECTOR	vectorized version routines	10
VIBANL	normal coordinate analysis	
VSCF	anharmonic frequencies	
ZAPDDI	distrib. data ZAPT2 open shell PT gradient	
ZHEEV	complex matrix diagonalization	
ZMATRX	internal coordinates	

UNIX versions use the C code ZUNIX.C for dynamic memory.

The machine dependencies noted above are:

- | | |
|--------------------------|-----------------------------|
| 1) packing/unpacking | 2) OPEN/CLOSE statements |
| 3) machine specification | 4) fix total dynamic memory |
| 5) subroutine walkback | 6) error handling calls |
| 7) timing calls | 8) LOGAND function |
| 10) vector library calls | 11) REAL*16 data type |

Note that the message passing support (DDI) for GAMESS is implemented in C (for most machines), and is stored in a separate subdirectory. Please see the ~/games/ddi tree for more information about the Distributed Data Interface's code and usage.

Programming Conventions

The following "rules" should be adhered to in making changes in GAMESS. These rules are important in maintaining portability, and should be adhered to.

The following rule is so important that it is not given a number,

The Golden Rule: make sure your code not only has no compiler diagnostics (try as many compilers as possible), but that it also has no FTNCHEK diagnostics. The FTNCHEK program of Robert Moniot is a fantastic debugging tool, and results in the great portability of GAMESS. You can learn how to get FTNCHEK, and how to use it from the script
~/gamess/misc/checkgms

Rule 1. If there is a way to do it that works on all computers, do it that way. Commenting out statements for the different types of computers should be your last resort. If it is necessary to add lines specific to your computer, PUT IN CODE FOR ALL OTHER SUPPORTED MACHINES. Even if you don't have access to all the types of supported hardware, you can look at the other machine specific examples found in GAMESS, or ask for help from someone who does understand the various machines. If a module does not already contain some machine specific statements (see the above list) be especially reluctant to introduce dependencies.

Rule 2. Write a double precision program, and let the source activator handle any conversion to single precision, when that is necessary:

a) Use IMPLICIT DOUBLE PRECISION(A-H,O-Z) specification statements throughout. Not REAL*8. Integer type should be just INTEGER, so that compiler flags can select 64 or 32 bit integers at compile time.

b) All floating point constants should be entered as if they were in double precision, in a format that the source code activator can recognize as being uniquely a number. Namely, the constants should contain a decimal point, a number after the decimal, and a signed, two digit exponent. A legal constant is 1.234D-02. Illegal examples are 1D+00, 5.0E+00, 3.0D-2. Check for illegals by

```
grep "[0-9][DE][0-9]" *.src
grep "[0-9][.]D" *.src
```

```
grep "[0-9][.][0-9][DE][0-9]" *.src  
grep "[0-9][DE][+][1-9][^0-9]" *.src
```

c) Double precision BLAS names are used throughout, for example DDOT instead of SDOT, and DGEMM instead of SGEMM.

The source code activator ACTVTE will automatically convert these double precision constructs into the correct single precision expressions for machines that have 64 rather than 32 bit words.

Rule 3. FORTRAN 77 allows for generic functions. Thus the routine SQRT should be used in place of DSQRT, as this will automatically be given the correct precision by the compilers. Use ABS, COS, INT, etc. Your compiler manual will tell you all the generic names.

Rule 4. Every routine in GAMESS begins with a card containing the name of the module and the routine. An example is "C*MODULE xxxxxx *DECK yyyyyy". The second star is in column 18. Here, xxxxxx is the name of the module, and yyyyyy is the name of the routine. This rule is designed to make it easier for a person completely unfamiliar with GAMESS to find routines.

Rule 5. Whenever a change is made to a module, this should be recorded at the top of the module. The information required is the date, initials of the person making the change, and a terse summary of the change.

Rule 6. No imbedded tabs, statements must lie between columns 7 and 72, etc. In other words, old style syntax.

* * *

The next few "rules" are not adhered to in all sections of GAMESS. Nonetheless they should be followed as much as possible, whether you are writing new code, or modifying an old section.

Rule 7. Stick to the FORTRAN naming convention for integer (I-N) and floating point variables (A-H, O-Z). If you've ever worked with a program that didn't obey this, you'll understand why.

Rule 8. Always use a dynamic memory allocation routine that calls the real routine. A good name for the memory

routine is to replace the last letter of the real routine with the letter M for memory.

Rule 9. All the usual good programming techniques, such as indented DO loops ending on CONTINUEs, IF-THEN-ELSE where this is clearer, 3 digit statement labels in ascending order, no three branch GO TO's, descriptive variable names, 4 digit FORMATs, etc, etc.

The next set of rules relates to coding practices which are necessary for the parallel version of GAMESS to function sensibly. They must be followed without exception!

Rule 10. All open, rewind, and close operations on sequential files must be performed with the subroutines SEQOPN, SEQREW, and SEQCLO respectively. You can find these routines in IOLIB, they are easy to use. SQREAD, SQWRIT, and various integral I/O routines like PREAD are used to process the contents of such files. The variable DSKWRK tells if you are processing a distributed file (one split between all compute processes, DSKWRK=.TRUE.) or a single file on the master node (DSKWRK=.FALSE., resulting in broadcasts of the data from the master to all other nodes).

Rule 11. All READ and WRITE statements for the formatted files 5, 6, 7 (variables IR, IW, IP, or named files INPUT, OUTPUT, PUNCH) must be performed only by the master task. Therefore, these statements must be enclosed in "IF (MASWRK) THEN" clauses. The MASWRK variable is found in the /PAR/ common block, and is true on the master process only. This avoids duplicate output from the other processes.

Rule 12. All error termination is done by "CALL ABRT" rather than a STOP statement. Since this subroutine never returns, it is OK to follow it with a STOP statement, as compilers may not be happy without a STOP as the final executable statment in a routine. The purpose of calling ABRT is to make sure that all parallel tasks get shut down properly.

Parallel broadcast identifiers

GAMESS uses DDI calls to pass messages between the parallel processes. Every message is identified by a unique number, hence the following list of how the numbers are used at present. If you need to add to these, look at the existing code and use the following numbers as guidelines to make your decision. All broadcast numbers must be between 1 and 32767.

20	:	Parallel timing
100 - 199	:	DICTIONRY file reads
200 - 204	:	Restart info from the DICTIONRY file
210 - 214	:	Pread
220 - 224	:	PKread
225	:	RAread
230	:	SQread
250 - 265	:	Nameio
275 - 310	:	Free format
325 - 329	:	\$PROP group input
350 - 354	:	\$VEC group input
400 - 424	:	\$GRAD group input
425 - 449	:	\$HESS group input
450 - 474	:	\$DIPDR group input
475 - 499	:	\$VIB group input
500 - 599	:	matrix utility routines
800 - 830	:	Orbital symmetry
900	:	ECP 1e- integrals
910	:	1e- integrals
920 - 975	:	EFP and SCRF integrals
980 - 999	:	property integrals
1000 - 1025	:	SCF wavefunctions
1030 - 1041	:	broadcasts in DFT
1050	:	Coulomb integrals
1200 - 1215	:	MP2
1300 - 1320	:	localization
1495 - 1499	:	reserved for Jim Shoemaker
1500	:	One-electron gradients
1505 - 1599	:	EFP and SCRF gradients
1600 - 1602	:	Two-electron gradients
1605 - 1620	:	One-electron hessians
1650 - 1665	:	Two-electron hessians
1700 - 1750	:	integral transformation
1800	:	GUGA sorting
1850 - 1865	:	GUGA CI diagonalization
1900 - 1910	:	GUGA DM2 generation
2000 - 2010	:	MCSCF

2100 - 2120 : coupled perturbed HF
2150 - 2200 : MCSCF hessian
2300 - 2309 : spin-orbit jobs

Disk files used by GAMESS

These files must be defined by your control language for executing GAMESS. For example, on UNIX the "name" field shown below should be set in the environment to the actual file name to be used. Most runs will open only a subset of the files shown below, with only files 5, 6, 7, and 10 used by every run. Files 2, 3, 4, 5, 6, 7, 35, and 36 contain formatted data, all others are binary (unformatted) files.

unit	name	contents
----	----	-----
2	ERICFMT	Fm(t) interpolation table data, data file ericfmt.dat supplied with GAMESS source.
3	MCCPATH	a directory of model core potentials and associated basis sets, supplied with the GAMESS source.
3	EXTBAS	external basis set library
4	IRCDATA	archive results punched by IRC runs, restart data for numerical HESSIAN runs, summary of results for DRC and for GLOBOP.
5	INPUT	Namelist input file. This MUST be a disk file, as GAMESS rewinds this file often.
6	OUTPUT	Print output (FT06F001 on IBM mainframes) If not defined, UNIX systems will use the standard output for this file.
7	PUNCH	Punch output. A copy of the \$DATA deck, orbitals for every geometry calculated, hessian matrix, normal modes from FORCE, properties output, IRC restart data, etc.
8	AOINTS	Two e- integrals in AO basis
9	MOINTS	Two e- integrals in MO basis
10	DICTNRY	Master dictionary, for contents see below.
11	DRTFILE	Distinct row table file for -CI- or -MCSCF-
12	CIVECTR	Eigenvector file for -CI- or -MCSCF-

13	CASINTS	semi-transformed ints for FOCAS/SOSCF MCSCF scratch file during spin-orbit coupling
14	CIINTS	Sorted integrals for -CI- or -MCSCF-
15	WORK15	GUGA loops for Hamiltonian diagonal; ordered two body density matrix for MCSCF; scratch storage during GUGA Davidson diag; Hessian update info during 2nd order SCF; [ij ab] integrals during MP2 gradient density matrices during determinant CI
16	WORK16	GUGA loops for Hamiltonian off-diagonal; unordered GUGA DM2 matrix for MCSCF; orbital hessian during MCSCF; orbital hessian for analytic hessian CPHF; orbital hessian during MP2 gradient CPHF; two body density during MP2 gradient
17	CSFSAVE	CSF data for state to state transition runs.
18	FOCKDER	derivative Fock matrices for analytic hess
19	WORK19	for code under development
20	DASORT	Sort file for various -MCSCF- or -CI- steps; also used by SCF level DIIS
21	DFTINTS	four center overlap ints for grid-free DFT
22	DFTGRID	mesh information for grid DFT
23	JKFILE	shell J, K, and Fock matrices for -GVB-; Hessian update info during SOSCF MCSCF; orbital gradient and hessian for QUAD MCSCF
24	ORDINT	sorted AO integrals; integral subsets during Morokuma analysis
25	EFPIND	electric field integrals for EFP
26	PCMDATA	gradient and D-inverse data for PCM runs
27	PCMINTS	normal projections of PCM field gradients
26	SVPWRK1	conjugate gradient solver for SV(P)SE
27	SVPWRK2	conjugate gradient solver for SV(P)SE

28	MLTPL	multipole moments of Gaussian basis function products during QFMM
29	MLTPLT	multipole moments of FMM boxes
30	DAFL30	direct access file for FOCAS MCSCF's DIIS; form factor sorting for Breit spin-orbit
31	SOINTX	Lx 2e- integrals during spin-orbit
32	SOINTY	Ly 2e- integrals during spin-orbit
33	SOINTZ	Lz 2e- integrals during spin-orbit
34	SORESC	RESC symmetrization of SO ints
35	SIMEN	GLOBOP simulated annealing energies
36	SIMCOR	GLOBOP simulated annealing coordinates
37	GCILIST	determinant list for general CI program
38	HESSIAN	hessian for FMO optimisations; gradient for FMO with restarts
40	SOCDDAT	CSF list for SOC; fragment densities/orbitals for FMO
41	AABB41	aabb spinor [ia jb] integrals during UMP2
42	BBAA42	baaa spinor [ia jb] integrals during UMP2
43	BBBB43	bbbb spinor [ia jb] integrals during UMP2

files 50-63 are used for MCQDPT runs.

unit	name	contents
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50	MCQD50	Direct access file for MCQDPT, its contents are documented in source code.
51	MCQD51	One-body coupling constants $\langle I/E_{ij}/J \rangle$ for CAS-CI and other routines
52	MCQD52	One-body coupling constants for perturb.
53	MCQD53	One-body coupling constants extracted from MCQD52
54	MCQD54	One-body coupling constants extracted further from MCQD52
55	MCQD55	Sorted 2e- AO integrals

56	MCQD56	Half transformed 2e- integrals
57	MCQD57	transformed 2e- integrals of (ii ii) type
58	MCQD58	transformed 2e- integrals of (ei ii) type
59	MCQD59	transformed 2e- integrals of (ei ei) type
60	MCQD60	2e- integral in MO basis arranged for perturbation calculations
61	MCQD61	One-body coupling constants between state and CSF $\langle \text{Alpha}/E_{ij}/J \rangle$
62	MCQD62	Two-body coupling constants between state and CSF $\langle \text{Alpha}/E_{ij},kl/J \rangle$
63	MCQD63	canonical Fock orbitals (FORMATTED)
64	MCQD64	Spin functions and orbital configuration functions (FORMATTED)
61	NMRINT1	derivative integrals for NMR
	...	
66	NMRINT6	" " " "
67	DCPHFH2	magnetic hessian in dynamic polarizability
68	DCPHF21	magnetic hessian times electronic hessian
69	GVVPT	for code under development

files 70-98 are used for Coupled-Clusters,
all of these are direct access files.

unit	name	contents
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70	CCREST	T1 and T2 amplitudes for restarting
71	CCDIIS	amplitude converger's scratch data
72	CCINTS	MO integrals sorted by classes
73	CCT1AMP	T1 amplitudes and some No*Nu intermediates for MMCC(2,3)
74	CCT2AMP	T2 amplitudes and some No**2 times Nu**2 intermediates for MMCC(2,3)
75	CCT3AMP	M3 moments
76	CCVM	No**3 times Nu - type main intermediate
77	CCVE	No times Nu**3 - type main intermediate
78	CCAUADS	Nu**3 times No intermediates for (TQ)
79	QUADSVO	No*Nu**2 times No intermediates for (TQ)
80	EOMSTAR	initial vectors for EOMCCSD calculations
81	EOMVEC1	iterative space for R1 components
82	EOMVEC2	iterative space for R2 components
83	EOMHC1	singly excited components of H-bar*R
84	EOMHC2	doubly excited components of H-bar*R
85	EOMHHHH	intermediate used by EOMCCSD
86	EOMPPPP	intermediate used by EOMCCSD
87	EOMRAMP	converged EOMCCSD right (R) amplitudes
88	EOMRTMP	converged EOMCCSD amplitudes for MEOM=2

(if the max. no. of iterations exceeded)

89	EOMDG12	diagonal part of H-bar
90	MMPP	diagonal parts for triples-triples H-bar
91	MMHPP	diagonal parts for triples-triples H-bar
92	MMCIVEC	Converged CISD vectors
93	MMCIVC1	Converged CISD vectors for mci=2 (if the max. no. of iterations exceeded)
94	MMCIITR	Iterative space in CISD calculations
95	EOMVL1	iterative space for L1 components
96	EOMVL2	iterative space for L2 components
97	EOMLVEC	converged EOMCCSD left eigenvectors
98	EOMHL1	singly excited components of L*H-bar
99	EOMHL2	doubly excited components of L*H-bar

201-239 OLI201 to OLI239 files used by RUNTYP=TDHFX

Contents of the direct access file 'DICTNRY'

1. Atomic coordinates
2. various energy quantities in /ENRGYS/
3. Gradient vector
4. Hessian (force constant) matrix
- 5-6. not used
7. PTR - symmetry transformation for p orbitals
8. DTR - symmetry transformation for d orbitals
9. FTR - symmetry transformation for f orbitals
10. GTR - symmetry transformation for g orbitals
11. Bare nucleus Hamiltonian integrals
12. Overlap integrals
13. Kinetic energy integrals
14. Alpha Fock matrix (current)
15. Alpha orbitals
16. Alpha density matrix
17. Alpha energies or occupation numbers
18. Beta Fock matrix (current)
19. Beta orbitals
20. Beta density matrix
21. Beta energies or occupation numbers
22. Error function interpolation table
23. Old alpha Fock matrix
24. Older alpha Fock matrix
25. Oldest alpha Fock matrix
26. Old beta Fock matrix
27. Older beta Fock matrix
28. Oldest beta Fock matrix
29. Vib 0 gradient in FORCE (numerical hessian)
30. Vib 0 alpha orbitals in FORCE
31. Vib 0 beta orbitals in FORCE
32. Vib 0 alpha density matrix in FORCE
33. Vib 0 beta density matrix in FORCE
34. dipole derivative tensor in FORCE.
35. frozen core Fock operator
36. Lagrangian multipliers
37. floating point part of common block /OPTGRD/
- int 38. integer part of common block /OPTGRD/
39. ZMAT of input internal coords
- int 40. IZMAT of input internal coords
41. B matrix of redundant internal coords
42. not used.
43. Force constant matrix in internal coordinates.
44. SALC transformation
45. symmetry adapted Q matrix
46. S matrix for symmetry coordinates

- 47. ZMAT for symmetry internal coords
- int 48. IZMAT for symmetry internal coords
- 49. B matrix
- 50. B inverse matrix
- 51. overlap matrix in Lowdin basis,
temp Fock matrix storage for ROHF
- 52. genuine MOPAC overlap matrix
- 53. MOPAC repulsion integrals
- 54. exchange integrals for screening
- 55. orbital gradient during SOSCF MCSCF
- 56. orbital displacement during SOSCF MCSCF
- 57. orbital hessian during SOSCF MCSCF
- 58. reserved for Pradipta
- 59. Coulomb integrals in Ruedenberg localizations
- 60. exchange integrals in Ruedenberg localizations
- 61. temp MO storage for GVB and ROHF-MP2
- 62. temp density for GVB
- 63. dS/dx matrix for hessians
- 64. dS/dy matrix for hessians
- 65. dS/dz matrix for hessians
- 66. derivative hamiltonian for OS-TCSCF hessians
- 67. partially formed EG and EH for hessians
- 68. MCSCF first order density in MO basis
- 69. alpha Lowdin populations
- 70. beta Lowdin populations
- 71. alpha orbitals during localization
- 72. beta orbitals during localization
- 73. alpha localization transformation
- 74. beta localization transformation
- 75. fitted EFP interfragment repulsion values
- 76. model core potential information
- 77. model core potential information
- 78. "Erep derivative" matrix associated with F-a terms
- 79. "Erep derivative" matrix associated with S-a terms
- 80. EFP 1-e Fock matrix including induced dipole terms
- 81. interfragment dispersion values
- 82. MO-based Fock matrix without any EFP contributions
- 83. LMO centroids of charge
- 84. d/dx dipole velocity integrals
- 85. d/dy dipole velocity integrals
- 86. d/dz dipole velocity integrals
- 87. unmodified h matrix during SCRF or EFP
- 88. PCM solvent operator contribution to Fock
- 89. EFP multipole contribution to one e- Fock matrix
- 90. ECP coefficients
- int 91. ECP labels
- 92. ECP coefficients
- int 93. ECP labels
- 94. bare nucleus Hamiltonian during FFIELD runs

- 95. x dipole integrals, in AO basis
- 96. y dipole integrals, in AO basis
- 97. z dipole integrals, in AO basis
- 98. former coords for Schlegel geometry search
- 99. former gradients for Schlegel geometry search
- 100. dispersion contribution to EFP gradient

records 101-248 are used for NLO properties

- | | | |
|----------------|-----------------------|----------------------|
| 101. U'x(0) | 149. U' 'xx(-2w;w,w) | 200. UM' 'xx(-w;w,0) |
| 102. y | 150. xy | 201. xy |
| 103. z | 151. xz | 202. xz |
| 104. G'x(0) | 152. yy | 203. yz |
| 105. y | 153. yz | 204. yy |
| 106. z | 154. zz | 205. yz |
| 107. U'x(w) | 155. G' 'xx(-2w;w,w) | 206. zx |
| 108. y | 156. xy | 207. zy |
| 109. z | 157. xz | 208. zz |
| 110. G'x(w) | 158. yy | 209. U' 'xx(0;w,-w) |
| 111. y | 159. yz | 210. xy |
| 112. z | 160. zz | 211. xz |
| 113. U'x(2w) | 161. e' 'xx(-2w;w,w) | 212. yz |
| 114. y | 162. xy | 213. yy |
| 115. z | 163. xz | 214. yz |
| 116. G'x(2w) | 164. yy | 215. zx |
| 117. y | 165. yz | 216. zy |
| 118. z | 166. zz | 217. zz |
| 119. U'x(3w) | 167. UM' 'xx(-2w;w,w) | 218. G' 'xx(0;w,-w) |
| 120. y | 168. xy | 219. xy |
| 121. z | 169. xz | 220. xz |
| 122. G'x(3w) | 170. yy | 221. yz |
| 123. y | 171. yz | 222. yy |
| 124. z | 172. zz | 223. yz |
| 125. U' 'xx(0) | 173. U' 'xx(-w;w,0) | 224. zx |
| 126. xy | 174. xy | 225. zy |
| 127. xz | 175. xz | 226. zz |
| 128. yy | 176. yz | 227. e' 'xx(0;w,-w) |
| 129. yz | 177. yy | 228. xy |
| 130. zz | 178. yz | 229. xz |
| 131. G' 'xx(0) | 179. zx | 230. yz |
| 132. xy | 180. zy | 231. yy |
| 133. xz | 181. zz | 232. yz |
| 134. yy | 182. G' 'xx(-w;w,0) | 233. zx |
| 135. yz | 183. xy | 234. zy |
| 136. zz | 184. xz | 235. zz |
| 137. e' 'xx(0) | 185. yz | 236. UM' 'xx(0;w,-w) |
| 138. xy | 186. yy | 237. xy |
| 139. xz | 187. yz | 238. xz |
| 140. yy | 188. zx | 239. yz |

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|------|------------|------|----------------|------|----|
| 141. | yz | 189. | zy | 240. | yy |
| 142. | zz | 190. | zz | 241. | yz |
| 143. | UM' 'xx(0) | 191. | e' 'xx(-w;w,0) | 242. | zx |
| 144. | xy | 192. | xy | 243. | zy |
| 145. | xz | 193. | xz | 244. | zz |
| 146. | yy | 194. | yz | | |
| 147. | yz | 195. | yy | | |
| 148. | zz | 196. | yz | | |
| | | 197. | zx | | |
| | | 198. | zy | | |
| | | 199. | zz | | |
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- 245. old NLO Fock matrix
 - 246. older NLO Fock matrix
 - 247. oldest NLO Fock matrix
 - 249. polarizability derivative tensor for Raman
 - 250. transition density matrix in AO basis
 - 251. static polarizability tensor alpha
 - 252. X dipole integrals in MO basis
 - 253. Y dipole integrals in MO basis
 - 254. Z dipole integrals in MO basis
 - 255. alpha MO symmetry labels
 - 256. beta MO symmetry labels
 - 257. not used
 - 258. Vnn gradient during MCSCF hessian
 - 259. core Hamiltonian from der.ints in MCSCF hessian
 - 260-261. reserved for Dan
 - 262. MO symmetry labels during determinant CI
 - 263. PCM nuclei/induced nuclear Charge operator
 - 264. PCM electron/induced nuclear Charge operator
 - 265. pristine alpha guess (MOREAD or Huckel+INSORB)
 - 266. EFP/PCM IFR sphere information
 - 267. fragment LMO expansions, for EFP Pauli
 - 268. fragment Fock operators, for EFP Pauli
 - 269-275. not used
 - 276. Vib 0 Q matrix in FORCE
 - 277. Vib 0 h integrals in FORCE
 - 278. Vib 0 S integrals in FORCE
 - 279. Vib 0 T integrals in FORCE
 - 280. Zero field LMOs during numerical polarizability
 - 281. Alpha zero field dens. during num. polarizability
 - 282. Beta zero field dens. during num. polarizability
 - 283. zero field Fock matrix. during num. polarizability
 - 284. Fock eigenvalues for multireference PT
 - 286. oriented localized molecular orbitals
 - 287. density matrix of oriented LMOs
 - 290-299. reserved for Alex Granovsky
 - 301. alpha Pocc during MP2/CIS grad (see also 361-369)
 - 302. alpha Pvir during MP2 gradient

- 303. alpha Wai during MP2 gradient
- 304. alpha Lagrangian Lai during MP2 or CI gradient
- 305. alpha Wocc during MP2 gradient
- 306. alpha Wvir during MP2 gradient
- 307. alpha P(MP2/CIS)-P(RHF) during MP2/CIS gradient
- 308. alpha SCF density during MP2 or CIS gradient
- 309. alpha energy weighted density in MP2 or CIS grad
- 311. Supermolecule h during Morokuma
- 312. Supermolecule S during Morokuma
- 313. Monomer 1 orbitals during Morokuma
- 314. Monomer 2 orbitals during Morokuma
- 315. combined monomer orbitals during Morokuma
- 316. RHF density in CI grad; nonorthog. MOs in SCF-MI
- 317. unzeroed Fock matrix when MOs are frozen
- 318. MOREAD orbitals when MOs are frozen
- 319. bare Hamiltonian without EFP contribution
- 320. MCSCF active orbital density
- 321. MCSCF DIIS error matrix
- 322. MCSCF orbital rotation indices
- 323. Hamiltonian matrix during QUAD MCSCF
- 324. MO symmetry labels during MCSCF
- 325. final uncanonicalized MCSCF orbitals
- 330. CEL matrix during PCM
- 331. VEF matrix during PCM
- 332. QEFF matrix during PCM
- 333. ELD matrix during PCM
- 340. DFT alpha Fock matrix
- 341. DFT beta Fock matrix
- 342. DFT screening integrals
- 343. DFT: V aux basis only
- 344. DFT density gradient d/dx integrals
- 345. DFT density gradient d/dy integrals
- 346. DFT density gradient d/dz integrals
- 347. DFT M[D] alpha density resolution in aux basis
- 348. DFT M[D] beta density resolution in aux basis
- 349. DFT orbital description
- 350. overlap of true and auxiliary DFT basis
- 351. previous iteration DFT alpha density
- 352. previous iteration DFT beta density
- 353. DFT screening matrix (true and aux basis)
- 354. DFT screening integrals (aux basis only)
- 355. h in MO basis during DDI partial transf
- 361-369. same as 301-309, but for beta orbitals of UMP2.
- 370. left transformation for pVp
- 371. right transformation for pVp
- 370. basis A (large component) during NESC
- 371. basis B (small component) during NESC
- 372. difference basis set A-B1 during NESC
- 373. basis N (rel. normalized large component)

- 374. basis B1 (small component) during NESC
- 375. charges of non-relativistic atoms in NESC
- 376. common nuclear charges for all NESC basis
- 377. common coordinates for all NESC basis
- 378. common exponent values for all NESC basis
- 372. left transformation for V during RESC
- 373. right transformation for V during RESC
- 374. 2T, T is kinetic energy integrals during RESC
- 375. pVp integrals during RESC
- 376. V integrals during RESC
- 377. Sd, overlap eigenvalues during RESC
- 378. V, overlap eigenvectors during RESC
- 379. Lz integrals
- 380. reserved for Ly integrals.
- 381. reserved for Lx integrals.
- 382. X, AO orthogonalisation matrix during RESC
- 383. Td, eigenvalues of 2T during RESC
- 384. U, eigenvectors of kinetic energy during RESC
- 385. exponents and contraction for the original basis
- int 386. shell integer arrays for the original basis
- 387. exponents and contraction for uncontracted basis
- int 388. shell integer arrays for the uncontracted basis
- 389. Transformation to contracted basis
- 390. S integrals in the internally uncontracted basis
- 391. charges of non-relativistic atoms in RESC
- 392. copy of one e- integrals in MO basis in SO-MCQDPT
- 393. Density average over all \$MCQD groups in SO-MCQDPT
- 394. overlap integrals in 128 bit precision
- 395. kinetic ints in 128 bit precision, for relativity

- 401. dynamic polarizability tensors

In order to correctly pass data between different machine types when running in parallel, it is required that a DAF record must contain only floating point values, or only integer values. No logical or Hollerith data may be stored. The final calling argument to DAWRIT and DAREAD must be 0 or 1 to indicate floating point or integer values are involved. The records containing integers are so marked in the list below.

Physical record 1 (containing the DAF directory) is written whenever a new record is added to the file. This is invisible to the programmer. The numbers shown above are "logical record numbers", and are the only thing that the programmer need be concerned with.