(30 December 2008)

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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:

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.

* * * * *

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     FORTRAN       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
CLENMO.*	cleans up $VEC groups
DK3.F	prepare relativistic AO contractions.

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

~/gamess/graphics

Better back-end graphics (3D as well as 2D) is available in the MacMolPlt program, now available for all popular desktop operating systems.

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 MWORDS 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 CPUs 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 CPUs. 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 original concept of distributed memory was implemented in the Global Array toolkit of Pacific Northwest National Laboratory (see http://www.emsl.pnl.gov/pub/docs/global).

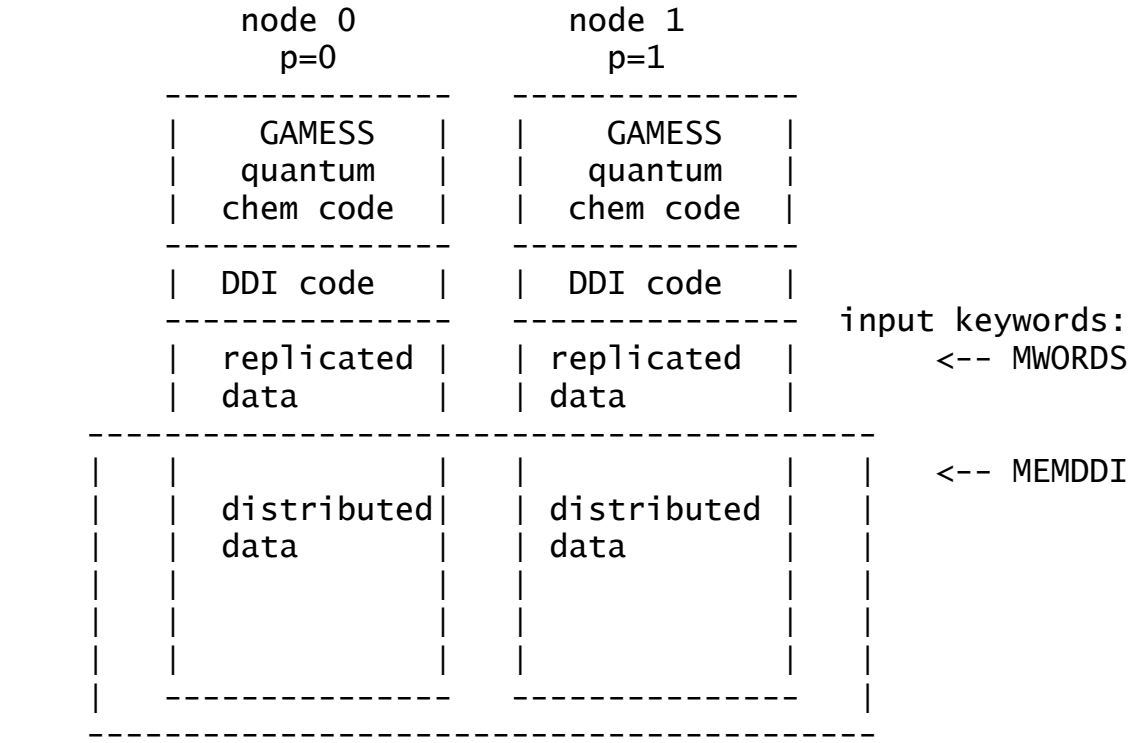
Basically, the idea is to provide three subroutine calls to access memory on other processors (in the local or even remote nodes): PUT, GET, and ACCUMULATE. These give access to a class of memory which is assumed to be slower than local memory, but faster than disk:

```
    <--- fastest                              slowest --->
 registers cache(s) local_memory remote_memory disks tapes
    <--- smallest                             biggest --->
```

Because DDI accesses memory on other CPUs by means of an explicit subroutine call, the programmer is aware that a message must be transmitted. This awareness of the access overhead should encourage algorithms that transfer many data items in a single message. Use of a subroutine call to reach remote memory is a recognition of the non-uniform memory access (NUMA) nature of parallel computers. In other words, the Distributed Data Interface (DDI) is an explicitly message passing implementation of global shared memory.

In order to have one CPU pass data items to a second CPU when the second CPU needs them, without significant delay, the computing job on the first CPU must interrupt its computation briefly to furnish the data. This type of communication is referred to as "one sided messages" or "active messages" since the first CPU is an unwitting participant in the process, which is driven entirely by the requirements of the second CPU.

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 processes (in this example, half on one and half on the other).

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

total on any 1 CPU = MWORDS + MEMDDI/p

Since MEMDDI is very large, its units are in millions of words. Since good execution speed requires that you not exceed the physical memory belonging to your CPUs, it is important to understand that when MEMDDI is large, you will need to choose a sufficiently large number of CPUs to keep the memory on each reasonable.

To repeat, the DDI philosophy is to add more processors not just for their compute performance or extra disk space,

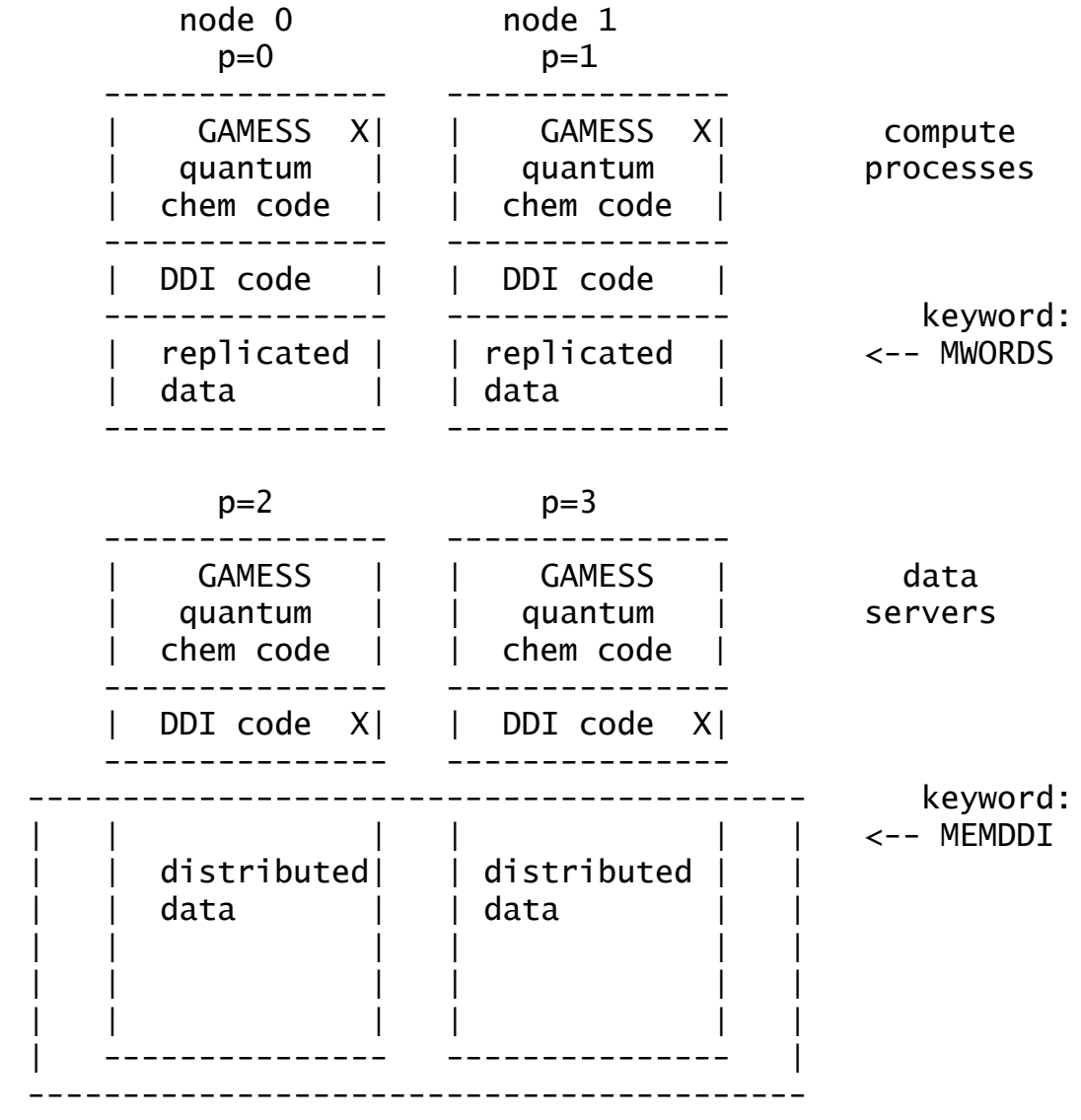
but also to aggregate a very large total memory. Bigger problems will require more CPUs to obtain sufficiently large total memories! We will give an example of how you can estimate the number of CPUs a little ways below.

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 interupt 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 CPU 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 CPU'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 interupts 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 process 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 CPU is unchanged, if p is the total number of CPUs used,

total on any 1 CPU = MWORDS + 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.

The parallel CCSD and CCSD(T) programs add a third kind of memory to the mix: node-replicated. This is data (e.g. the doubles amplitudes) that is stored only once per node. Thus, this is more copies of the data than once per parallel job (fully distributed MEMDDI) but fewer than once per CPU (replicated MWORDS). A picture of the memory model for the CCSD(T) program can be found in the "readme.ddi" file, so is not duplicated here. There is presently no keyword for this type of memory, but the system limit on the total SystemV memory does apply. It is important to perform a check run when using CCSD(T) and carefully follow the printout of its memory requirements.

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 CPU in the MWORDS (or the older keyword MEMORY in $SYSTEM) 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, and how to compute how many CPUs are needed to do the run.

Check runs (EXETYP=CHECK) need to run quickly, and the fastest turn around always comes on one CPU only. Runs which do not currently exploit MEMDDI distributed storage will formally allocate their MWORDS needs, and feel out their storage needs while skipping almost all of the real work. Since MWORDS is replicated, the amount that is needed on 1 CPU remains unchanged if you later do the true computation on more than 1 CPU.

Check jobs which involve MEMDDI storage are a little bit trickier. As noted, we want to run on only 1 CPU to get fast turn around. However, MEMDDI is typically a large amount of memory, and this is unlikely to be available on a single CPU. The solution is that the check job will 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 1024 MB of memory per processor, or some similar very large number. Let us say that a closed shell MP2 check run for this case gives the output of

```
  SCALED *PER-NODE* MEMORY REQUIREMENT
  NODES  DISTRIBUTED/MWORDS  REPLICATED/WORDS TOTAL/MBYTES
    1         952                 7284508          7624
```

The real run requires MWORDS=8 MEMDDI=960. Note that we have just rounded up a bit from the 7.3 and 952 in this output, for safety.

Of course, the actual computation will have to run on a large number of such processors, because you don't have 8 GB on your CPU, we are assuming 1024 MB (1 GB). Let us continue to compute how many processors are needed. We need to reserve some memory for the operating system (25 MB, say) and for the GAMESS program and local storage (let us say 50 MB, for GAMESS is a big program, and the compute processes should be swapped into memory). Thus our hypothetical 1024 MB processor has 950 MB available, assuming no one else is running. In units of words, this machine has 950/8 = 118 million words available for your run. We must choose the number of processors p to satisfy

needed <= available

```
      MWORDS + MEMDDI/p <= free physical memory
              8 + 960/p <= 118
```

so solving for p, we learn this example requires p >= 9 compute processes. The answer for roughly 8 GB of distributed memory on 1 GB processors was not 8, because the O/S, GAMESS itself, and the MWORDS requirements together mean less than 1 GB could be contributed to the distributed total. More CPUs than 9 do not require changing MWORDS or MEMDDI, but will run faster than 9. Fewer CPUs than 9 do not have enough memory to run!

One more subtle point about CHECK runs with MEMDDI is that since you are running on 1 CPU 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 keyword 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 DOORDO, PARAIO, 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 CPUs can be efficiently used for various SCFTYP and RUNTYP jobs

The performance data you will see below were obtained on a 16 CPU Intel Pentium II Linux (Beowulf-type) cluster costing $49,000, of which $3,000 went into the switched

Fast Ethernet component. 512 MB/CPU means this cluster has an aggregate memory of 8 GB. For more details, see
http://www.msg.chem.iastate.edu/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 CPU 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 AO 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 implimented, see the main GAMESS paper,

M.W.Schmidt, K.K.Baldridge, 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 C11O4H10, 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/CPU 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 CPUs 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 processors, 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 CPU 0. Since the integral transformation is run in replicated MWORDS memory, rather than distributing this, and since it also needs a duplicated AO integral file be

stored on every CPU, 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	
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 more or less serial here. This data comes from before the ALDET and ORMAS codes were given a replicated memory parallization, so scaling in the CI step should now be OK, to say 8 or 16 CPUs. However, these two CI code's use of replicated memory in the CI step limits MCSCF scalability in the large active space limit.

Now let's consider the second order pertubation 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 processor. However, some things can be run only on 1 CPU, 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 processors 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 CPUs (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/gamess/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 basis functions, and reducing the storage for the effective fragment and PCM solvent models.

Of course, the 'mung' script can also be used to increase the dimensions!

To fully turn off effective fragment storage, use MXFRG=4, MXDFG=1, MXPT=8, MXFGPT=4. To fully turn off PCM storage, use MXSP=1, MXTS=1. 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.
Reducing the storage size makes sense mainly on microkernel
type systems, without virtual memory managers.

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 tesserae 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	
BASG3L	G3Large 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	
CCDDI	parallel CCSD(T) program	
CCQAUX	auxiliaries for CCSD(TQ) program	
CCQUAD	renormalized CCSD(TQ) corrections	
CCSDT	renormalized CCSD(T) program	1
CEEIS	corr. energy extrap. by intrinsic scaling	
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
DCCC	divide and conquer coupled cluster	
DCGUES	divide and conquer orbital guess	
DCINT2	divide and conquer AO integrals	1
DCLIB	divide and conquer library routines	
DCMP2	divide and conquer MP2	1
DCSCF	divide and conquer SCF	
DCTRAN	divide and conquer integral transf.	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
DFTDIS   empirical dispersion correction to DFT
DFTFUN   grid-free DFT functionals
DFTGRD   grid DFT implementation
DFTINT   grid-free DFT integrals                1
DFTXCA   grid DFT functionals, hand coded
DFTXCB   grid DFT functionals, from repository
DFTXCC   grid DFT functionals for meta-GGA
DFTXCD   grid DFT functionals B97, etc
DFTXCE   grid DFT functionals for PKZB/TPSS family
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
EFPFMO   FMO and EFP interface
EIGEN    Givens-Householder, Jacobi diagonalization
ELGLIB   elongation method utility routines
ELGLOC   elongation method orbital localization
ELGSCF   elongation method Hartree-Fock         1
EOMCC    equation of motion excited state CCSD
EWALD    Ewald summations for EFP model
FFIELD   finite field polarizabilitie
FMO      n-mer drivers for Fragment Molecular Orbital
FMOESD   elestrostatic potential derivatives for FMO
FMOGRD   gradient routines for FMO
FMOINT   integrals for FMO
FMOIO    input/output and printing for FMO
FMOLIB   utilities for FMO
FMOPBC   periodic boundary conditions for FMO
FMOPRP   properties for FMO
FRFMT    free format input scanner
FSODCI   determinant based second order CI
```

G3	G3(MP2,CCSD(T)) thermochemistry	
GAMESS	main program, important driver routines	
GLOBOP	Monte Carlo fragment global optimizer	
GMCPT	general MCQDPT multireference PT code	1
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	11
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
IVOCAS	improved virtual orbital CAS energy	1
LAGRAN	CI Lagrangian matrix	1
LOCAL	various localization methods	1
LOCCD	LCD SCF localization analysis	
LOCPOL	LCD SCF polarizability analysis	1
MCCAS	FOCAS/SOSCF MCSCF calculation	1
MCJAC	JACOBI MCSCF calculation	
MCPGRD	model core potential nuclear gradient	

```
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
MEXING   minimum energy crossing point search
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
MP2GR2   disk based MP2 gradient program
MP2IMS   disk based MP2 energy program
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   dummy routines for NEO program
NMR      nuclear magnetic resonance shifts       1
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     dummy routines for Tinker/SIMOMM program
QREL     relativistic transformations
RAMAN    Raman intensity
RHFUHF   RHF, UHF, and ROHF HF-SCF                1
ROHFCC   open shell CC computations               1
RXNCRD   intrinsic reaction coordinate
RYSPOL   roots for Rys polynomials
SCFLIB   HF-SCF utility routines, DIIS code
SCFMI    molecular interaction SCF code
SCRF     self consistent reaction field
SOBRT    full Breit-Pauli spin-orbit compling
SOFFAC   spin-orbit matrix element form factors
SOLIB    spin-orbit library routines
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      "        "         "
TDDEFP   EFP solvent effects on TD-DFT
TDDFT    time-dependent DFT excitations
TDDFUN   functionals for TD-DFT
TDDFXC   exchange-corr. grid pts. for TD-DFT
TDDGRD   gradient code for TD-DFT
TDDINT   integral terms for TD-DFT                1
TDDXCA   functional derivatives for TD-DFT
TDHF     time-dependent Hartree-Fock polarzblity 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
UTDDFT   unrestricted TD-DFT                       1
VBDUM    dummy routines for VB programs
VECTOR   vectorized version routines              10
VIBANL   normal coordinate analysis
VSCF     anharmonic frequencies
VVOS     valence virtual orbitals
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 statments
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 souce 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 process (DSKWRK=.FALSE., resulting in broadcasts of the data from the master to all other CPUs).

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     : DICTNRY file reads
 200 -  204     : Restart info from the DICTNRY 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 in order to execute 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 1, 2, 3 (both), 4, 5, 6, 7, and 35 contain formatted data, while all others are binary (unformatted) files. Files ERICFMT, EXTBAS, and MCPPATH are used to read data into GAMESS. Files MAKEFP, TRAJECT, RESTART, and PUNCH are supplemental output files, containing more concise summaries than the log file for certain kinds of data.

unit	name	contents
1	MAKEFP	effective fragment potential from MAKEFP run
2	ERICFMT	Fm(t) interpolation table data, a data file named ericfmt.dat, supplied with GAMESS.
3	MCPPATH	a directory of model core potentials and associated basis sets, supplied with GAMESS
3	EXTBAS	external basis set library (user supplied)
3	GAMMA	3rd nuclear derivatives
4	TRAJECT	trajectory results for IRC, DRC, or MD runs. summary of results for RUNTYP=GLOBOP.
35	RESTART	restart data for numerical HESSIAN runs, numerical gradients, or for RUNTYP=VSCF. Used as a scratch unit during MAKEFP.
5	INPUT	Namelist input file. This MUST be a disk file, as GAMESS rewinds this file often.
6	OUTPUT	Print output (main log file). If not defined, UNIX systems will use the file "standard output" for this.
7	PUNCH	Punch output. A copy of the $DATA deck, orbitals for every geometry calculated, hessian matrix, normal modes from FORCE, properties output, etc. etc. 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	used during CP-MCHF response equations
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,
               direct access file for NEO's nuclear DIIS,
               direct access file for DC'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   RESTART, documented at the beginning of this list

37   GCILIST   determinant list for general CI program

38   HESSIAN   hessian for FMO optimisations;
               gradient for FMO with restarts

39   QMMTEI    reserved for future use

40   SOCCDAT   CSF list for SOC;
               fragment densities/orbitals for FMO

41   AABB41    aabb spinor [ia|jb] integrals during UMP2

42   BBAA42    bbaa spinor [ia|jb] integrals during UMP2

43   BBBB43    bbbb spinor [ia|jb] integrals during UMP2


     files 50-63 are used for MCQDPT runs.
```

```
     files 50-54 are also used by CODE=IMS MP2 runs.

unit  name     contents
----  ----     --------
50    MCQD50   Direct access file for MCQDPT, its
               contents are documented in source code.
51    MCQD51   One-body coupling constants <I/Eij/J> 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 <Alpha/Eij/J>
62    MCQD62   Two-body coupling constants between state
               and CSF <Alpha/Eij,kl/J>
63    MCQD63   canonical Fock orbitals  (FORMATTED)
64    MCQD64   Spin functions and orbital configuration
               functions (FORMATTED)


unit  name     contents
----  ----     --------
        for RUNTYP=NMR only
61    NMRINT1  derivative integrals for NMR
62    NMRINT2      "         "       "   "
63    NMRINT3      "         "       "   "
64    NMRINT4      "         "       "   "
65    NMRINT5      "         "       "   "
66    NMRINT6      "         "       "   "
        for RUNTYP=MAKEFP (or dynamic polarizability run)
67    DCPHFH2  magnetic hessian in dynamic polarizability
68    DCPHF21  magnetic hessian times electronic hessian
        for NEO runs, only (DAFL30 has nuclear DIIS)
67    ELNUINT  electron-nucleus AO integrals
68    NUNUINT  nucleus-nucleus AO integrals
69    NUMOIN   nucleus-nucleus MO integrals
70    NUMOCAS  nucleus-nucleus half transformed integrals
71    NUELMO   nucleus-electron MO integrals
72    NUELCAS  nucleus-electron half transformed integrals
        for elongation method, only
```

70	ELGDOS	elongation density of states
71	ELGDAT	elongation frozen/active region data
72	ELGPAR	elongation geometry optimization info
74	ELGCUT	elongation cutoff information
75	ELGVEC	elongation localized orbitals
77	ELINTA	elongation 2e- for cut-off part
78	EGINTB	elongation 2e- for next elongation
79	EGTDHF	elongation TDHF (future use)
80	EGTEST	elongation test file

files 70-98 are used for closed shell Coupled-Cluster, all of these are direct access files.

unit	name	contents
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

the next group of files (70-95) is for open shell CC:

unit  name     contents
----  ----     --------
70   AMPROCC   restart CCSD/Lambda equation information
71   ITOPNCC   working copy of the same information
72   FOCKMTX   subsets of F-alpha and F-beta matrices
73   LAMB23    data during CC(2,3) step
74   VHHAA     [i,k|j,l]-[i,l|j,k] alpha/alpha
75   VHHBB     [i,k|j,l]-[i,l|j,k] beta/beta
76   VHHAB     [i,k|j,l] alpha/beta
77   VMAA      [j,l|k,a]-[j,a|k,l] alpha/alpha
78   VMBB      [j,l|k,a]-[j,a|k,l] beta/beta
79   VMAB      [j,l|k,a] alpha/beta
80   VMBA      [j,l|k,a] beta/alpha
81   VHPRAA    [a,j|c,l]-[a,l|c,j] alpha/alpha
82   VHPRBB    [a,j|c,l]-[a,l|c,j] beta/beta
83   VHPRAB    [a,j|b,l] alpha/beta
84   VHPLAA    [a,b|k,l]-[a,l|b,k] alpha/alpha
85   VHPLBB    [a,b|k,l]-[a,l|b,k] beta/beta
86   VHPLAB    [a,b|k,l] alpha/beta
87   VHPLBA    [a,b|k,l] beta/alpha
88   VEAA      [a,b|c,l]-[a,l|b,c] alpha/alpha
89   VEBB      [a,b|c,l]-[a,l|b,c] beta/beta
90   VEAB      [a,j|c,d] alpha/beta
91   VEBA      [a,j|c,d] beta/alpha
92   VPPPP    all four virtual integrals
93   INTERM1  one H-bar, some two H-bar, etc.
94   INTERM2  some two H-bar, etc.
95   INTERM3  remaining two H-bar intermediates


unit  name     contents
----  ----     --------
         files 201-239 may be used by RUNTYP=TDHFX
201   OLI201...running consecutively up to
239   OLI239
         files 250-257 are used by divide-and-conquer runs
         file 30 is used for the DC-DIIS data
250   DCSUB    subsystem atoms (central and buffer)
251   DCVEC    subsystem orbitals
252   DCEIG    subsystem eigenvalues
253   DCDM     subsystem density matrices
254   DCDMO    old subsystem density matrices
255   DCQ      subsystem Q matrices
256   DCW      subsystem orbital weights
257   DCEDM    subsystem energy-weighted density matrices
```

```
   files 297-299 are used by hyperpolarizability analysis
297   LHYPWRK  preordered LMOs
298   LHYPKW2  reassigned LMOs
299   BONDDPF  bond dipoles with electric fields
```

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. RHF/UHF/ROHF Lagrangian (see 402-404)
    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
```

```
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

    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
269-270. not used
    271. orbital density matrix in divide and conquer
int 272. subsystem data during divide and conquer
273-275. 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. not used
    301. Pocc during MP2 (RHF or ZAPT) or CIS grad
    302. Pvir during MP2 gradient (UMP2= 411-429)
    303. Wai during MP2 gradient
    304. Lagrangian Lai during MP2 gradient
    305. Wocc during MP2 gradient
    306. Wvir during MP2 gradient
    307. P(MP2/CIS)-P(RHF) during MP2 or CIS gradient
    308. SCF density during MP2 or CIS gradient
    309. energy weighted density in MP2 or CIS gradient
    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
    334. PVE tesselation info during PCM
335-339. not used
    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 integral transformation
    356. alpha symmetry MO irrep numbers if UHF/ROHF
    357. beta  symmetry MO irrep numbers if UHF/ROHF
```

```
358-369. not used
    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
396-400. not used
    401. dynamic polarizability tensors
    402. GVB Lagrangian
    403. MCSCF Lagrangian
    404. GUGA CI Lagrangian (see 308 for CIS)
    405. not used
    406. MEX search state 1 alpha orbitals
    407. MEX search state 1 beta orbitals
    408. MEX search state 2 alpha orbitals
    409. MEX search state 2 beta orbitals
    410. not used
    411. alpha Pocc during UMP2 gradient (see 301-309)
    412. alpha Pvir during UMP2 gradient
```

```
    413. alpha Wai during UMP2 gradient
    414. alpha Lagrangian Lai during UMP2 gradient
    415. alpha Wocc during UMP2 gradient
    416. alpha Wvir during UMP2 gradient
    417. alpha P(MP2/CIS)-P(RHF) during UMP2 gradient
    418. alpha SCF density during UMP2 gradient
    419. alpha energy weighted density in UMP2 gradient
    420. not used
421-429. same as 411-419, for beta orbitals
    430. not used
440-469. reserved for NEO
    470. QUAMBO expansion matrix
    471. excitation vectors for FMO-TDDFT
    472. X+Y in MO basis during TD-DFT gradient
    473. X-Y in MO basis during TD-DFT gradient
    474. X+Y in AO basis during TD-DFT gradient
    475. X-Y in AO basis during TD-DFT gradient
    476. excited state density during TD-DFT gradient
    477. energy-weighted density in AO basis for TD-DFT
478-490. not used
    491. gradients vectors during NACME
    492. NACME vectors during NACME
493-950. not used
```

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.