

Computing for Science (CFS) Ltd.,  
CCLRC Daresbury Laboratory.

Generalised Atomic and Molecular Electronic Structure System

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# G A M E S S - U K

## USER'S GUIDE and REFERENCE MANUAL

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PART 1. INTRODUCTION and GENERAL FEATURES

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## Introduction to GAMESS-UK

GAMESS-UK is a general purpose *ab initio* molecular electronic structure program for performing SCF-, DFT- and MCSCF-gradient calculations, together with a variety of techniques for post Hartree Fock calculations.

The program is derived from the original GAMESS code, obtained from Michel Dupuis in 1981 (then at the National Resource for Computational Chemistry, NRCC), and has been extensively modified and enhanced over the past decade. This work has included contributions from numerous authors (see below), and has been conducted largely at the former EPSRC (Engineering and Physical Sciences Research Council), and now CCLRC Daresbury Laboratory, under the auspices of Collaborative Computational Project No. 1 (CCP1). Other major sources that have assisted in the on-going development and support of the program include various academic funding agencies in the Netherlands, and ICI plc.

All publications resulting from use of this program must include the following acknowledgement:

*GAMESS-UK is a package of ab initio programs. See: <http://www.cfs.dl.ac.uk/gamess-uk/index.shtml>, M.F. Guest, I. J. Bush, H.J.J. van Dam, P. Sherwood, J.M.H. Thomas, J.H. van Lenthe, R.W.A. Havenith, J. Kendrick, "The GAMESS-UK electronic structure package: algorithms, developments and applications", *Molecular Physics*, Vol. 103, No. 6-8, 20 March-20 April 2005, 719-747, doi:[10.1080/00268970512331340592](https://doi.org/10.1080/00268970512331340592).*

Depending on which modules are used, the following references should be cited:

- MCSCF/CASSCF:  
P.J. Knowles, G.J. Sexton and N.C. Handy, *Chem. Phys.* 72 (1982) 337, doi:[10.1016/0301-0104\(82\)85131-8](https://doi.org/10.1016/0301-0104(82)85131-8):  
P.J. Knowles and H.-J. Werner, *Chem. Phys. Lett.* 115 (1985) 259, doi:[10.1016/0009-2614\(85\)80025-7](https://doi.org/10.1016/0009-2614(85)80025-7).
- MØLLER-PLESSET PERTURBATION THEORY (MP2, MP3):  
J.E. Rice, R.D. Amos, N.C. Handy, T.J. Lee and H.F. Schaefer, *J. Chem. Phys.* 85 (1986) 963, doi:[10.1063/1.451253](https://doi.org/10.1063/1.451253):  
J.D. Watts and M. Dupuis, *J. Comput. Chem.* 9 (1988) 158, doi:[10.1002/jcc.540090208](https://doi.org/10.1002/jcc.540090208).
- FULL CI (FCI):  
S. Zarrabian and R.J. Harrison, *Chem. Phys. Letts.* 81 (1989), doi:[10.1016/0009-2614\(89\)87358-0](https://doi.org/10.1016/0009-2614(89)87358-0)
- DIRECT-CI (DCI):  
V.R. Saunders and J.H. van Lenthe, *Mol. Phys.* 48 (1983) 923, doi:[10.1080/00268978300100661](https://doi.org/10.1080/00268978300100661).
- CONVENTIONAL CI (MRDCI):  
R.J. Buenker in 'Studies in Physical and Theoretical Chemistry', 21 (1982) 17.
- MULTIPLE ACTIVE SPACE SCF (MASSCF):  
J. Ivanić, *J. Chem. Phys.* 119, 9364-9376(2003), doi:[10.1063/1.1615954](https://doi.org/10.1063/1.1615954).
- DISTRIBUTED MULTIPOLE ANALYSIS (DMA):  
A.J. Stone, *Chem. Phys. Letters* 83 (1981) 233, doi:[10.1016/0009-2614\(81\)85452-8](https://doi.org/10.1016/0009-2614(81)85452-8).
- OUTER-VALENCE GREENS' FUNCTION (OVGF):  
L.S. Cederbaum and W. Domcke, *Adv. Chem. Phys.* 36 (1977) 205.
- TAMM-DANCOFF METHOD (TDA):  
J. Schirmer and L.S. Cederbaum, *J. Phys.* B11 (1978) 1889:  
I.H. Hillier, K. Rigby, M. Vincent, M.F. Guest and W. von Niessen, *Chem. Phys. Lett.* 134 (1987) 403, doi:[10.1016/0009-2614\(87\)87162-2](https://doi.org/10.1016/0009-2614(87)87162-2).
- EFFECTIVE CORE POTENTIALS (LOCAL ECPs):  
P.J. Hay and W.R. Wadt, *J. Chem. Phys.* 82 (1985) 270, 284, 299, doi:[10.1063/1.448800](https://doi.org/10.1063/1.448800).

- EFFECTIVE CORE POTENTIALS (NON-LOCAL ECPS):  
Ph. Durand and J.-C. Berthelat, *Theoret. Chim. Acta*, 38 (1975) 283, doi:[10.1007/BF00963468](https://doi.org/10.1007/BF00963468):  
N.A. Burton, I.H. Hillier, M.F. Guest and J. Kendrick, *Chem. Phys. Lett.* 155 (1989) 195, doi:[10.1016/0009-2614\(89\)85348-5](https://doi.org/10.1016/0009-2614(89)85348-5)].
- INFRA-RED AND RAMAN INTENSITIES:  
R.D. Amos, *Adv. Chem. Phys.* 67 (1987) 99, doi:[10.1002/9780470142936.ch2](https://doi.org/10.1002/9780470142936.ch2).
- MULTI CONFIGURATION LINEAR RESPONSE (MCLR):  
C. Fuchs, V. Bonačić-Koutecký and J. Koutecký, *J. Chem. Phys.* 98 (1993) 3121, doi:[10.1063/1.464086](https://doi.org/10.1063/1.464086).
- COUPLED CLUSTER CCSD AND CCSD(T):  
T.J. Lee, J.E. Rice and A.P. Rendell, *The TITAN Set of Electronic Structure Programs*, 1991,
- DENSITY FUNCTIONAL THEORY (DFT):  
The initial DFT module within GAMESS-UK was developed by Dr. P. Young under the auspices of EPSRC's Collaborative Computational Project No. 1 (CCP1) (1995-1997). Subsequent developments have been undertaken by staff at the Daresbury Laboratory.
- DIRECT REACTION FIELD (DRF):  
A.H. de Vries, P.Th. van Duijnen, A.H. Juffer, J.A.C. Rullmann, J.P. Dijkman, H. Merenga, and B.T. Thole, *J. Comp. Chem.* 16 (1995) 37–55, doi:[10.1002/jcc.540160105](https://doi.org/10.1002/jcc.540160105) erratum 1445–1446, doi:[10.1002/jcc.540161113](https://doi.org/10.1002/jcc.540161113); P.Th. van Duijnen and A.H. de Vries, *Int. J. Quant. Chem.*, 60 (1996) 1111, doi:[10.1002/\(SICI\)1097-461X\(1996\)60:6;1111::AID-QUA2;3.0.CO;2-2](https://doi.org/10.1002/(SICI)1097-461X(1996)60:6;1111::AID-QUA2;3.0.CO;2-2);

Additional key references and background material on each of the modules are provided at appropriate points throughout this manual.

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## 1 About This Manual

This manual is divided into sixteen parts or 'chapters', which may be broadly classified as follows:

- *Part 1 (this part)* describes the general features of the program, detailing the file system employed and the directive structure associated with the free-format data input.
- *Part 2* presents a series of example data files designed to provide a broad outline of the various capabilities of the program. Subsequent chapters provide a more detailed description of the data input formats.
- *Parts 3 and 4* describe the directives required in performing SCF, Møller Plesset, CASSCF, MCSCF, DFT and associated gradient calculations.
- *Part 5* deals with integral transformation and Direct-CI calculations.
- *Part 6* covers conventional and semi-direct Table-CI calculations.
- *Part 7* describes the data required in performing RPA and MCLR calculations.
- *Part 8* describes the various analysis capabilities of the code, plus the directives and scope of the DRF solvation module.
- *Part 9* presents a brief summary of possible problem areas in running the code.
- *Part 10* provides a brief summary of the utility functions associated with GAMESS-UK.
- *Part 11* describes the way formatted output may be obtained from GAMESS-UK for use by other programs.
- *Part 12* presents a sequence of worked examples on a UNIX machine, using the specially provided script *rungames*
- *Part 13* provides a series of worked examples invoking the GAMESS-UK binary directory from a UNIX shell (C-shell).
- *Part 14* describes the capabilities and running of the parallel version of GAMESS-UK on both MPP and SMP hardware.
- *Turtle* describes how to run the GAMESS-UK Valence Bond module.
- *Mopac* describes the GAMESS-UK/MOPAC interface.

The user who wishes to acquire rapid familiarity and a sufficient subset of knowledge to use the program, albeit perhaps in a somewhat restricted fashion, should concentrate initially on Parts 1 and 2, together with any appropriate examples from Parts 12-14.

The example input files described in Part 2 are supplied with GAMESS-UK and can be found in the scripts labelled c2001\_a - c2035 in the directory: **GAMESS-UK/examples/chap2**.

NB: this documentation describes features available in the current release of the code (Version 8.0); some of the features described herein may not function as described in earlier releases of the program.

## 2 General Features

GAMESS-UK [1] is a general purpose *ab initio* molecular electronic structure program for performing SCF-, DFT- and MCSCF-gradient calculations, together with a variety of techniques for post Hartree Fock calculations. On-going development of the code is co-ordinated from Daresbury, with the program currently available on a wide range of machines, including:

- a wide variety of UNIX workstations, including those from SGI (R4000-, R4400-, R8k- and R10k-Indigo<sup>2</sup>, R5k-, R10k- and R12k-O2, Challenge and Power Challenge, Origin200, Origin2000, Origin300 and Origin3800), Hewlett Packard (Model 9000/7xx, PA8000, PA8200, PA8500, PA8600 and PA8700), IBM RS/6000s (PowerPC, Power1, Power2, P2SC, Power3, Power4 and Power5), Compaq/Digital (EV5-, EV6-, EV67- and EV68-AXP under Tru64, OSF/1, OpenVMS and Linux), and SUN (Super-, Hyper- and Ultra-SPARC);
- a number of IA-32, IA-64 and AMD PCs (e.g. Pentium, PentiumII, Pentium III, Pentium 4, Xeon, EM64T, Itanium1 and Itanium2, Athlon and Opteron) under Linux, FreeBSD and Windows NT, 2000 and XP;
- Mac OSX running on Power 3, 4 and 5 processors.
- Parallel versions of the code are available on both MPP and SMP platforms. MPP versions include those for the IBM p-series (TN2, P2SC, WH2 and Regatta nodes), and a variety of IA32, IA64, EM64T, AMD64 and Alpha-based Beowulf Systems. SMP versions are available for the SGI Origin and Altix, Compaq AlphaServer SC and Cray XD1. Ports to the Fujitsu VPP300 and NEC SX-5 are also available.
- Versions for other machines of mainly historical interest include the Intel iPSC/860, Amdahl VP, IBM-3090/VF, Convex C2 and C3 series, and Kendall Square KSR-2, Cray Y-MP, C90 and J90, T3D and T3E (Cray-T3E/900 and Cray/T3E-1200), VAX VMS and Hitachi SR2201.

The program utilises the Rys Polynomial or Rotation techniques [2] to evaluate repulsion integrals over s,p,d,f and g type Cartesian Gaussian orbitals. Open- and closed-shell SCF treatments are available within both the RHF and UHF framework, with convergence controls provided through a hybrid scheme of level shifters and the DIIS method [3]. In addition generalised valence bond [4], complete active space SCF [5] and more general MCSCF [6], MASSCF [8] and Møller Plesset (MP2 and MP3) [7] calculations may be performed. The original limitation to cartesian basis sets is lifted through the provision of spherical harmonic basis sets for all options within the programme. The most recent additions to the code, available from Version 6.0 onwards, include a full-featured Density Functional Theory (DFT) module, with access to a wide variety of functionals (S-VWN, B-LYP, B-P86, B3-LYP, HCTH, B97, B97-1, B97-2, FT97 etc). This module is subject to on-going developments under the auspices of CCP1.

The analytic energy gradient is available for each class of wavefunction above. Gradients for s and p Gaussians are evaluated using the algorithm due to Schlegel [9], while gradients involving d, f and g Gaussians utilise the Rys Polynomial Method.

Geometry optimisation may be carried out using the DL-FIND module that is included into GAMESS-UK (see Part 4 for information about DL-FIND).

Alternatively, GAMESS-UK has its own optimisation capabilities using a quasi-Newton rank-2 update method, while transition state location is available through either a synchronous transit [10], trust region [11] or 'hill-walking' [12, 13] method. Force constants may be evaluated analytically [14] and by numerical differentiation; coupled Hartree-Fock (CHF) calculations provide for a range of molecular properties, including polarisabilities and molecular hyperpolarisabilities [15] and, through the calculation of dipole moment and polarisability derivatives, the computation of infra-red and Raman intensities [16].

*Ab initio* core potentials are provided in both semi-local [17] and non-local [18] formalism for valence-only molecular orbital treatments.

Conventional CI treatments using the table-driven selection algorithms within the framework of MR-DCI calculations [19] have been extended to include an implementation of the semi-direct table-driven MRDCI module. This provides more extensive capabilities in the treatment of electronic spectra and related phenomena. The variety of correlation treatments available include Direct-CI [20], Full-CI [21], and both CCSD [22, 23] and CCSD(T) [24, 25] coupled-cluster calculations, the latter being limited to closed-shell systems [26]. A size-consistent variant of Multi-Reference MP2 theory, popularized in its CASPT2 form by Roos et al., is also available [35]. With no restriction to CAS wavefunctions, the module also provides MR-MP3 capabilities.

The direct calculation of molecular valence ionization energies may be performed through Green's function techniques, using either the outer-valence Green's function (OVGF) [27] or the two-particle-hole Tamm-Dancoff method (2ph-TDA) [28].

Calculations of electronic transition energies and corresponding oscillator strengths may also be performed using either the Random Phase Approximation (RPA) method or the Multiconfigurational Linear Response (MCLR) procedure [29]. The RPA calculations may be performed either within the conventional approach where the two-electron integrals are transformed or with a "direct" implementation.

A variety of wavefunction analysis methods are provided, including population analysis, Natural Bond Orbital (NBO) [30] and distributed multipole analysis [32], localised orbitals, graphical analysis and calculation of 1-electron properties. An interface to the AIMPAC code of Bader is provided [31] for SCF, DFT, MCSCF, MP2, MP3, MRDCI and Direct-CI calculations.

The treatment of solvation effects is now based on the DRF (Direct Reaction Field) model [33, 34], an embedding technique enabling the computation of the interaction between a quantum-mechanically described molecule and its classically described surroundings. The classical surroundings may be modelled in a number of ways, (i) by point charges to model the electrostatic field due to the surroundings (ii) by polarizabilities to model the (electronic) response of the surroundings (iii) by an enveloping dielectric to model bulk response (both static and electronic) of the surroundings, and (iv) by an enveloping ionic solution, characterized by its Debye screening length.

The treatment of relativistic effects is provided within the ZORA scheme (Zeroth Order Regular Approximation [36]), a two component alternative to the full 4 component Dirac equation.

While much cheaper than the latter, ZORA recovers a large part of the relativistic effects. The scalar (1-component) form is now available, with the full 2-component implementation (including spin-orbit coupling) in progress. The current implementation will allow all usual *Ab Initio* (and DFT) methods to be performed, incorporating the major relativistic effects.

The restriction of a maximum of 255 basis functions when performing conventional processing of two-electron integrals has been removed in nearly all modules in Version 7.0 of the code. The program structure is open-ended in both direct-SCF, -DFT and direct-MP2 mode, so that direct-SCF calculations up to 22,000 basis functions have been performed. Version 7.0 also features a significant extension to the parallel capabilities of GAMESS-UK.

In addition to the functionality outlined above, the program provides for (i) Hybrid QM/MM calculations, through an interface to the CHARMM QM/MM code, developed in collaboration with B. Brooks and E. Billings, of the NIH, and (ii) a Utilities module concerned with house-keeping, library file creation, file manipulation etc.

The program also includes version 7.0 of the MOPAC [38] semi-empirical code, enabling the calculations with the semi-empirical Hamiltonians MNDO, MINDO/3, AM1, PM3, PM5, and MNDO-d. The interface between GAMESS-UK and MOPAC allows coordinates calculated with MOPAC to be imported into GAMESS-UK for a subsequent *ab initio* calculation.

A free Graphical User Interface (the CCP1GUI) has also been developed to simplify the use of the code and to graphically display the results of calculations. Further information on the CCP1GUI, as well as downloadable packages for a number of different operating systems can be found on the web at:

<http://www.cse.scitech.ac.uk/ccg/software/ccp1gui/>

Areas of application for GAMESS-UK include:

- Theoretical studies of reaction surfaces. SCF and MCSCF calculations of equilibrium and transition state geometries, and the evaluation of force constants and vibrational frequencies at these stationary points.
- Energy assignments in the entire field of electronic spectroscopy. Calculation of spectroscopic properties of highly excited molecular and ionic states. Evaluation of transition moments.
- Graphical and numerical analysis of Hartree Fock and post-Hartree Fock wavefunctions.
- Generation of zero-order wavefunctions required in the more extensive treatments of dynamical correlation energy. Applicability to general systems with many electrons in this treatment of dynamical correlation energy. Benchmark treatments of correlation energy using Full-CI calculations.
- Theoretical mechanistic studies of chemisorption in heterogeneous catalysis.
- Treatment of bio-organic and related molecules through Direct-SCF calculations and electrostatic potential analysis.



## 3 Units used in the manual

Throughout the manual, use is made of the units of "words" and "blocks" to describe the sizes of files and/or memory. These are defined as follows:

### 3.1 WORD

A word is defined as a FORTRAN DOUBLE PRECISION or INTEGER\*8 datatype and is 8 bytes (64 bits) long.

### 3.2 BLOCK

The definition of BLOCK is derived from the ATMOL [37] file system, where a BLOCK is 512 words (4096 bytes) long.

## 4 The File System

In this section we provide a brief overview of the file system used by GAMESS-UK. Note at this stage that both direct access and FORTRAN sequential data sets may be used by the program, the exact usage being a function of the particular activity in hand. Manipulation of these files e.g., keeping, deleting etc is described in the "pre-directives" section of Part 3 of this manual and also under the *rungamess* script in Part 13.

### 4.1 Direct Access Data Sets

Extensive use is made of the system of disk and tape handling originally developed within the ATMOL [37] program system, with the various files of integral data output to one or more direct access data sets. Such data sets are allocated to the program using logical file names (LFNs) in the range ED0, ED1, ..., ED19 and MT0, MT1, ..., MT19. In Table 1 we list those files used by the program, and define the default LFN associated with each file. A full description of data set management will not be given here: for the present it suffices to note the following;

1. The Dumpfile, which in default is routed to ED3, is crucial to the program and controls all restart activities. This file is organised into variable length sections, with the user nominating various sections for data storage e.g., eigenvectors. The sections are characterised by integers (in the range 1 - 350), which are specified by the user through data input.
2. The Scratchfile, which is routed to ED7, is used in all runs of the program as a file for house-keeping activities. While this data set need never be maintained across separate runs of the program, the user should be aware of the role of ED7 and avoid any attempts to use the data set in, for example, the re-routing of integral output.

3. Each data file is block addressable (1 block = 512 words). In default output of each file commences at block 1 of the associated data set, and continues in uninterrupted fashion until output is complete. With certain exceptions, the user may control file usage in several ways;
  - redefine the LFN to be associated with a given data file
  - redefine the starting block for the file, allowing several files of data to be stored on the same data set
  - partition output of a given file over several data sets, specifying the associated LFNs, and the starting and terminal blocks of each LFN. This feature is particularly useful in controlling the output of two-electron integrals. It is not possible, however, to fragment the Dumpfile, Scratchfile or Direct-CI file.
  - while mainly of historical interest, we note that direct access files needed, on an IBM Mainframe (running the MVS or VM/CMS operating system), to be preallocated. This process assumed the user had some idea of the overall space requirements, since any attempt to route file output beyond the terminal block of a preallocated file was viewed as an unrecoverable error condition. Preallocation was not required when using the more-restrictive sequential data sets, which may be accessed though the LFNs MT0-MT19. Note that these considerations refer only to GAMESS-UK usage on an IBM mainframe. On other machines no formal distinction is made between direct (ED0-ED19) and sequential (MT0-MT19) files.

## 4.2 FORTRAN Data Sets

In addition to the direct access data sets described above GAMESS-UK will, in certain phases of computation e.g., Table-CI, make use of the more conventional FORTRAN unformatted sequential data sets. In the majority of cases this usage is restricted to scratch activities, and the user need not be concerned with, for example, FORTRAN unit specification. In some instances, however, it may be necessary to 'keep' the files in question between jobs. This activity should be controlled through the appropriate FILE pre-directives (see Part 3 of this manual).

## 5 Data Input - The Directive Structure

Data input for GAMESS-UK consists of a sequence of data lines, where a GAMESS-UK data line consists of a number of data fields, the fields being separated by at least one space character. The separating spaces are not considered part of the data field.

### 5.1 Data Lines

Data lines normally end at column 72, assuming a 'carriage return' is used as the line terminator (although this can be altered by means of the pre-directive WIDTH (see Part 3 of this manual). In fact there are several valid terminators recognised for a data line. These include

Table 1: Direct Access Files and Default LFNs used by GAMESS-UK

File	Contents	Default LFN
Mainfile	Two-electron integrals	ED2
Dumpfile	Eigenvectors, restart information	ED3
Scratchfile	Hessians, CI-coefficients etc Temporary file for program housekeeping	ED7
Libraryfile	Pseudopotential Library File	ED0
Symmetry Adapted Mainfile	Two-electron integrals in a symmetry adapted basis	ED1
Secondary Mainfile	Partially transformed two-electron integrals	ED4
Direct-CI file	Direct-CI file for restarts and symbolic hamiltonian etc	ED5
Transformed Integral File	Transformed two-electron integrals	ED6
Overflow file	Direct-CI file for symbolic hamiltonian	ED8
Loop Formulae Tape	Symbolic formulae used in CASSCF	ED9
Reordered Formulae Tape	Reordered symbolic formulae	ED10
Density Matrix File	Two particle density matrix used in CASSCF geometry optimisation	ED11
Hamiltonian File	Derivative Fock Operators	ED12
Reordered Integral File	Reordered two-electron integrals used in MCSCF	ED13
Scratchfiles	Temporary files used in derivative integral calculations	ED16-ED19
Sortfile	Temporary file for sorting integrals	SORT
P-Sortfile	Temporary file for sorting molecular integrals	PSORT
Tablefile	Table-CI file for storing data-base of pattern matrix elements	TABLE

- the conventional 'carriage-return' (CR).
- the back-slash character (\).
- the colon character (:)

Thus the following sequence of data lines

```
TITLE
H2CO - 3-21G DEFAULT BASIS - CLOSED SHELL SCF
ZMATRIX ANGSTROM
C
O 1 1.203
H 1 1.099 2 121.8
H 1 1.099 2 121.8 3 180.0
END
ENTER
```

could be presented as:

```
TITLE\H2CO - 3-21G DEFAULT BASIS - CLOSED SHELL SCF
ZMATRIX ANGSTROM\C\O 1 1.203\H 1 1.099 2 121.8
H 1 1.099 2 121.8 3 180.0\END
ENTER
```

Note also that a data line with one of the characters #, > or < in the first column will be treated by the program as 'comment' lines, being merely echoed to the output file. It goes without saying that the \ character should be avoided in any TITLE data.

## 5.2 Data Fields

A data field consists of a succession of non-space characters on a single line. Three types of field are in use:

- *A-fields* are used for the introduction of textual material, in the form of character strings. The maximum length of an A-field is 8 characters. A-fields of less than 8 characters are padded to the right with spaces, while if more than 8 characters are found, the field is truncated from the right, so that only the leftmost 8 characters are significant.
- *I-fields* are used for the introduction of numeric data in the form of integers, and consist of a succession of decimal digits possibly preceded by a + or - sign. The sign character may be omitted, when the integer is assumed to be positive. The following are examples of valid I-fields:

```
0
762
+4033
-6149
```

- *F-fields* are used for the input of floating point numbers. They are as *I-fields* except that a 'decimal point' character may appear to the right of the sign character. To introduce a decimal exponent a concatenation of a *F-field*, followed by the character *E* or *D*, followed by an *I-field*, without intervening blanks is allowed. The following are equivalent *F-fields*:

0      .0      0.      0.0      +0.0

as are:

0.0003      3E-4      3D-4      0.3E-3      +30E-5

and:

-500.0      -500      -5E2      -5E+2      -5D+2

Format descriptors are used to describe a data line. The simplest of these takes the form *nA*, or *nI* or *nF*, where *n* is a decimal integer. Thus the format *nF* describes a line consisting of *n* successive *F-fields*. The omission of the integer (*n*) before a letter code implies that *n*=1. More complicated descriptors are used; for example (*iA, jI, kF*) describes a line consisting of *i* *A-fields*, followed by *j* *I-fields*, followed by *k* *F-fields*. Consider the following line:

ATOM 10 1.0 12 HCH

read to the variables *TEXT, I, X, J, BTEXT* in format (*A, I, F, I, A*).

- *TEXT* will be set to the character string *ATOM*.
- *I* will be set to the decimal integer 10.
- *X* will be set to the floating point value 1.0.
- *J* will be set to the decimal integer 12.
- *BTEXT* will be set to the character string *HCH*.

The same line could be read to variables *TEXT, X, Y, ATEXT, BTEXT* in format (*A, 2F, 2A*), so that:

- *TEXT* will be set to the character string *ATOM*.
- *X* will be set to the floating point value 10.0.
- *Y* will be set to the floating point value 1.0.
- *ATEXT* will be set to the character string 12.
- *BTEXT* will be set to the character string *HCH*.

Consider reading the following line:

```
GENERALISED ATOMIC AND MOLECULAR ELECTRONIC STRUCTURE SYSTEM
```

to (A(l),l=1,7) in format (7A).

- A(1) will be set to the string GENERALI. Note the truncation.
- A(2) will be set to the string ATOMIC.
- A(3) will be set to the string AND.
- A(4) will be set to the string MOLECULA. Note the truncation.
- A(5) will be set to the string ELECTRON. Note the truncation.
- A(6) will be set to the string STRUCTUR. Note the truncation.
- A(7) will be set to the string SYSTEM.

### 5.3 GAMESS-UK Directives

Data input is largely structured as a sequence of 'directives'. Directives sometimes extend over many lines, sometimes they comprise a single line, and usually contain some reasonably self-contained data, built up out of A, I, and/or F-fields. The first field of a directive is invariably an A-field, carrying the name of the directive. Note that only the first four characters of such an identifier are in practice required. The directives group into two classes, with *Class 1* directives (see Part 3) specified before *Class 2* directives (see Part 4); note that the order within each class may be important, and the user is recommended to follow the order outlined in the relevant sections of the manuals, or example inputs where available.

#### 5.3.1 INCLUDE - Including external files in an input file

As of version 7.0 it is possible to include external text files into a GAMESS-UK input file through the use of the 'include' directive. Thus the line:

```
include /home/wab/inputs/geometry.txt
```

placed in a GAMESS-UK input file would cause the "geometry.txt" file to be inserted at that point in the input file.

## 6 Restrictions

The restrictions which the present program place on the user are as follows

- Gaussian functions of s, p, d, f and g may be used.

- The maximum number of contracted orbitals depends in general on the functionality requested. Conventional SCF and DFT energy and gradient calculations are now effectively open-ended (the default being 1024 functions). Note that lifting this restriction to an arbitrary number is trivially performed by changing the build size when configuring the code.
- The maximum number of primitive functions within a contraction is 25.
- The maximum number of centres is 1000, allowing for the use of extensive point-charge arrays.

## 7 Release Notes for GAMESS-UK

### 7.1 Changes introduced in GAMESS-UK Version 7.0

#### 7.1.1 Changes to GAMESS-UK functionality

##### 1. Fermi-dirac smearing implemented

Normally orbitals are filled according to a step function, but this can cause convergence problems if it is uncertain which state to converge on. Fermi smearing allows orbitals to be partially filled, which can improve convergence in some problematic cases.

##### 2. Atomic Guess extended

It is now possible to specify the per-atom electron configuration or charge for the atomic guess. It is also possible to specify alpha and beta populations for atoms in UHF calculations.

##### 3. Update of the Graphics Module

The graphics modules have been revised to enable both density and potential codes to drive through full (s,p,d,f,g) basis sets.

##### 4. User-defined convergence schemes:

It is now possible for a user to specify a particular convergence scheme, rather than the default one within GAMESS-UK. This is activated by placing the convergence criteria within a block in the input file delimited by the keywords "newscf" and "end", following the specification of the runtime.

This functionality is available in serial and within the parallel MPI ScaLAPACK driver.

##### 5. Changes to the DFT Module

- New DFT Functionals Several new functionals have been added:
  - PBE exchange-correlation functional
  - HCTH120, HCTH147, HCTH407, KT1 and KT2 functionals.
  - PW92 local correlation functional

- PW91 exchange, correlation and exchange-correlation functionals.
- B95 meta-GGA correlation functional.
- BB95, B1B95 and BB1K meta-GGA functionals. NB - for the meta-GGA functionals, only the energies and gradients can be calculated - the second derivatives of the energy are not available.
- More flexible DFT grid specifications
 

The atom size is used in a number of tests within in the DFT code. Previously the same size was used for all tests, however it is now possible to specify the atomic size for each test separately, as shown in the examples below:

  - (a) The atomic radii for the angular grid pruning schemes: pradii 3.0
  - (b) The atomic size adjustment radii for the weighting scheme: wradii 3.0
  - (c) The screening radius: sradii 3.0
  - (d) The radial grid scale factor: radii 3.0

It is also now possible to specify the grid size for a row of the periodic table - previously this had to be done on a per-element basis. For example, to specify the grid size for the Lebedev-Laikov angular grid for the first row of the periodic table: lebedev row 1 194

## 6. Changes to the Post-HF Modules

- The 255 basis function limit in the MRDCI code has been removed, so that the code is effectively open-ended in the number of basis functions permitted.
- Configuration Interaction Transformation between AO and MO basis' has been extended to g functions.
- A facility to allow the punching of both transformed integrals and CI coefficients from the full CI code has been introduced. This uses (i) the cards directive, and (ii) an extension of the current print facility within the Full CI module. Thus the data file:

```

core 10000000
title
h2co - 3-21g basis - valence full-ci
super off nosym
cards trans fullci
zmatrix angstrom
c
o 1 1.203
h 1 1.099 2 121.8
h 1 1.099 2 121.8 3 180.0
end
active\5 to 22 end\core\1 to 4\end
runtype ci\fullci 18 4 4
punch 1 -8
enter

```

Would result in a complete list of transformed 1e- and 2e-integrals to the file "moints,ascii" and all ci coefficients (greater than  $1 * 10^{*-8}$ ) to the file civecs.ascii.



- The filenames for the files use in CI calculations can now be set through "file" directives in the input file as well as environment variables.
  - MR-ACPF (Multireference Averaged Coupled-Pair-Functional), MR-AQCC (Multi-Reference Average Quadratic Coupled-Cluster) and the CEPA0 coupled electron-pair approximation methods have been added to the MRDCI module.
7. The use of the "HARMONIC" directive has been extended to the Valence Bond code, allowing spherical harmonic basis sets to be used for d, f and g functions.
  8. A simple solvation model has been implemented in the Valence Bond code.
  9. Arbitrary (not spinadapted) wavefunctions are now possible in the Valence Bond code.
  10. The Valence Bond module can be compiled with 8-byte integers.
  11. The "RESTORE" option has been added to the ZORA module to allow zora relativistic (atomic) corrections to be stored and restored on the current and foreign dumpfile. This permits easy restart calculations, when the ZORA corrections do not need to be recalculated.
  12. New distributed data MPI HF/DFT driver

A distributed-data HF and DFT module has been developed using MPI-based tools such as ScaLAPACK. All data structures, except those required for the Fock build are fully distributed. The functionality of this code is currently limited to closed shell and unrestricted open shell. To build this code BLACS and ScaLAPACK (available from <http://www.netlib.org/>), must be installed on the target machine and the "mpi" build option selected when configuring the code.
  13. Taskfarming Harness

A taskfarming harness has been developed. This is an MPI program designed to be run on a large number of processors on a parallel machine and 'batch processes' numerous small GAMESS-UK jobs. The taskfarming harness is currently only available as a separate binary of the "mpi" build of the code and is selected by choosing the "taskfarm" keyword when configuring the mpi code.

### 7.1.2 Changes to the structure of the code

#### 1. New Ports

The code has been ported to several new platforms:

- Macintosh OSX (G3, G4, and G5 processors)
- Windows XP
- AMD Opteron and Athlon processors running Linux.
- Intel Xeon, EM64T and Itanium processors running Linux.
- HP-UX running on Itanium processors.

- Sunfire v880 server
  - SGI Altix
  - Cray XD1
2. Global Arrays  
The version of the Global Arrays supplied with GAMESS-UK has been updated from 3.3 to GA 3.4b.
  3. MOPAC  
The MOPAC code within GAMESS-UK has been updated to version 7.0
  4. Configuring GAMESS-UK  
A new configure process has been developed to ease porting the code to new platforms and making it easier for users to configure the build on their own machine. All platform-specific variables for the make process are stored in a file with an .mk suffix in the **GAMESS-UK/config** directory and the configuration process is run by the configure script in the main **GAMESS-UK** directory. There are further notes in the file: **GAMESS-UK/INSTALL**.

### 7.1.3 Peripheral Changes

1. Demo Binaries  
Free Windows, Macintosh and Linux demo versions are available for users who wish to try out the code.
2. Changes to the website  
The website has been updated and moved to a new url and a Bugzilla facility for logging and querying bugs with the code has also been added.  
The new URL for the main GAMESS-UK website is:  
<http://www.cfs.dl.ac.uk>
3. CCP1GUI  
The CCP1GUI is a free, extensible Graphical User Interface to various computational chemistry codes. Although it has interfaces to other codes such as Dalton and Mopac, the CCP1GUI has been developed around GAMESS-UK and provides a powerful tool for setting up and viewing the results of calculations with GAMESS-UK.  
The CCP1GUI website can be found at:  
<http://www.cse.scitech.ac.uk/ccg/software/ccp1gui>

## 7.2 Changes introduced in GAMESS-UK Version 6.3

1. Section numbers for vectors/enter can now be omitted.
2. DMA analysis now uses Slater radii table.

3. The old option of performing a DFT energy calculation on a HF density (a posteriori) is no longer in the default build. This can still be accessed using the old-dft keyword in the configure response at build time.
4. Changes to the DFT module:
  - More flexible grid input.
  - Additional DFT functionals (FT97, HCTH, B97, B97-1 and B97-2 etc.)
  - Optimisations to coulomb fit DFT code.
  - Built-in DFT Orbital sets (DZVP, DZVP2 and TZVP) and Auxiliary Coulomb Fitting Basis sets (DGauss-A1 and -A2, DeMon and those due to Ahlrichs).
  - Gradient term from derivative of quadrature weights included.
5. Reduced functionality build options (SCF+DFT and MP2) for use on parallel machines with limited node memory, and for benchmark porting exercises.
6. Major changes to all ECP-related code. with re-writes of the integrals and derivatives code. This has sped the energy integrals by between 2-3, and the gradients by a factor of at least 5. Addition of 4 sets of ECPs to internal libraries
  - LANL2 (including all inner-valence TM ECPs etc to library; the original HW ECP's are now code-named lanl)
  - CRENBS and CRENBL (Christiansen et al Small- and Large-core ECPs)
  - STRLC and STRSC (Stuttgart RLC and RSC sets)all ECPs + associated basis sets added for all elements.
7. New Ports
  - Linux PowerPC
  - Windows95
  - Parallel version for Alpha/Linux clusters.
  - 64-bit build supported on a range of platforms (Origin, Alpha Linux, AIX, Solaris)
8. Global Array and Peigs source for parallel builds has been updated, supporting a wider range of platforms.
9. Ability to read in hessian information under runtime optx.
10. Ability to use include directive in input files.
11. Extensions/enhancements to ZORA.
12. Alpha release of Multi-Reference Moller Plesset module.
13. NBO analysis extended to UHF wavefunctions. Interface provided to Bader's AIMPAC code.

14. Alpha release of newscf module allowing more flexible treatment of cases showing poor SCF convergence.
15. Reduction in memory usage for systems with many nuclear centres, e.g. for QM/MM studies.
16. Developments to support VB code (under development, not included in Release 6.3.1)
17. Work on CHARMM interface code.

### 7.3 Changes introduced in GAMESS-UK Version 6.2

1. New functionality available includes;
  - Alpha release of Direct Reaction Field module.
  - Gaussian functions of s, p, d, f and g may now be used
  - Alpha release of ZORA Relativistic treatment.
  - Production release of Density Functional Theory (DFT) module.
  - Alpha release of semi-direct Table-CI module.
2. Change to the default behaviour of the DFT module  
Users of alpha-releases of the DFT module should note that now
  - the default functional is now B-LYP
  - the default grids are now constructed from the logarithmic grid of Knowles and Mura (previously the SG1 grid was selected by default).
3. Point charge calculations using BQ centres - the nuclear energy now excludes the term arising from BQ-BQ interactions. This should simplify the construction of QM/MM models by allowing the classical electrostatic energy to be computed entirely within the MM code. The original behaviour may be restored with the BQBQ directive.

## 8 Enquiries

All enquiries regarding the availability of the program documented herein, should be directed in the first instance to the following E-Mail address at Daresbury: [gamess.uk\\_contact@dl.ac.uk](mailto:gamess.uk_contact@dl.ac.uk)

For any problems arising from use of the program, there are two sources of help.

- There is a bug tracker that lists known problems with the code, which can be found at:  
[http://ccpforge.cse.rl.ac.uk/tracker/?group\\_id=14](http://ccpforge.cse.rl.ac.uk/tracker/?group_id=14)
- The gamess-uk-users email list is the place to raise any queries about the code or to ask for advice on using the code. The homepage for the list can be found at:  
<http://ccpforge.cse.rl.ac.uk/mailman/listinfo/gamess-uk-users>

Note that an electronic copy of this manual is available under the CFS web pages: <http://www.cfs.ac.uk/docs/index.shtml>

## 9 Acknowledgement

This program resulted from the efforts of many researchers: we gratefully acknowledge the on-going collaborative efforts of those colleagues detailed in the preface to this manual.

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