Outline

- Program Capabilities
- Input
- Output
- Memory and Processor usage
- Visualization
GAMESS

- Program primarily for wave-based modeling of the electronic structure of chemical systems.
Runs on...

- Any UNIX-type operating system
  - GAMESS Nov 22-04 is installed on the Power4/regatta
  - March-06 is installed on the Altix
  - March-07-r1 is installed on the BladeCenter
  - March-07-r1 is installed on Calhoun

- Most recent version (March 07-R6) also runs under CygWin on Windows
- A native Windows version is also maintained at Moscow State University
Theory available

- Hartree-Fock, Density functional theory
- Møller-Plesset perturbation theory (MP2)
- Configuration interaction (CI, FCI)
- Coupled-cluster calculations
  - CCSD[T], CCSD(T), CR-CCSD(T)
- Semi-empirical (AM1, PM3)
Basis sets

- Many basis sets available with keywords, others can be read in from the input.
Calculations types

- Geometry optimization
- TS search
- Find Minimum energy path for reaction
- Frequency calculations
Input File Format

- Input is arranged into groups. Each group begins with the group name and ends with $END. For example:
All valid input

$SCF    DIRSCF=.TRUE.    $END

$SCF

$END

$SCF

DIRSCF=.TRUE.

$END
Column 1 must be blank

$SCF    DIRSCF=.TRUE.    $END

$SCF    $END

BLANK

$SCF

$END

$SCF    DIRSCF=.TRUE.    $END
• Each group has a number of switches or variables set. The proper format depends on the group.

• $\text{DATA}$ is the only group required

• $\text{CONTRL}$ and $\text{SYSTEM}$ are almost always used.
$BASIS

GBASIS=N311 NGAUSS=6 NDFUNC=1

$END

Allows you to choose from standard basis sets.

This example specifies a 6-311G(d) basis set.
Non-standard basis sets can be read in the $DATA group.
$DATA group

$DATA
My CCSD(T) calculation

<table>
<thead>
<tr>
<th>C</th>
<th>6.0</th>
<th>0.00</th>
<th>0.00</th>
<th>0.00</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>6.0</td>
<td>1.25</td>
<td>0.71</td>
<td>0.00</td>
</tr>
<tr>
<td>H</td>
<td>1.0</td>
<td>0.28</td>
<td>2.27</td>
<td>0.00</td>
</tr>
</tbody>
</table>

$END
$DATA group

$DATA
My CCSD(T) calculation

CN 1

Symmetry group

C1, CS, CI, CN, S2N, CNH, CNV, DN, DNH, DND, T, TH, TD, O, OH
$DATA group

$DATA
My CCSD(T) calculation

CN 1

Symmetry

N is this number

Symmetry group

C1, CS, CI, CN, S2N, CNH, CNV, DN, DNH, DND, T, TH, TD, O, OH
$DATA group

$DATA
My CCSD(T) calculation

CN 1

Symmetry

Highest rotational axis
$DATA group

$DATA
My CCSD(T) calculation
DNH 4

Symmetry

If the system is linear, choose D4H symmetry.
### $DATA group

$DATA
My CCSD(T) calculation
CN 1

<p>| | | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>6.0</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>C</td>
<td>6.0</td>
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<td>0.00</td>
</tr>
<tr>
<td>H</td>
<td>1.0</td>
<td>0.28</td>
<td>2.27</td>
<td>0.00</td>
</tr>
</tbody>
</table>

$END
$DATA group

<p>| | | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>C</strong></td>
<td>6.0</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td><strong>C</strong></td>
<td>6.0</td>
<td>1.25</td>
<td>0.71</td>
<td>0.00</td>
</tr>
<tr>
<td><strong>H</strong></td>
<td>1.0</td>
<td>0.28</td>
<td>2.27</td>
<td>0.00</td>
</tr>
</tbody>
</table>

$END
$DATA group

$DATA
C 6.0 0.0 0.0 0.0 0.0
D 1
1 0.626 1.00
F 1
1 0.8000 1.00
...
$END

Specifying a General basis set
$DATA group

$DATA
C  6.0 0.0 0.0 0.0 0.0
D  1
  1   0.626   1.00
F  1
  1   0.8000  1.00
...
$END

Download any basis set in this format from the EMSL basis set library
$CONTROL$

- **Set level of theory**
  - SCF type (RHF, ROHF, UHF)
  - Correlation energy (MP2, CCSD, ...)
- **Set calculation type**
  - Energy
  - Geometry optimization
  - Frequency calculation
$CONTRL

  RUNTYP=ENERGY
  COORD=ZMT
  SCFTYP=RHF
  CITYP=ALDET

$END

Controls the basic Calculation being performed
$CONTRL

RUNTYP=ENERGY
COORD=ZMT
SCFTYP=RHF
CITYP=ALDET
$END

Single energy calculation
$CONTRL

RUNTYP=ENERGY
COORD=ZMT
SCFTYP=RHF
CITYP=ALDET

$END

Read in geometry assuming a z-matrix format
$CONTRL

RUNTYP=ENERGY
COORD=ZMT
SCFTYP=RHF
CITYP=ALDET

Restricted Hartree-Fock SCF for reference function

$END
$CONTRL

RUNTYP=ENERGY
COORD=ZMT
SCFTYP=RHF
CITYP=ALDET

$END

Ames Laboratory Determinant Full CI package
When this is set, GAMESS will look for the $CIDET group in the input file.
Two more $CONTRL examples

$CONTRL
  RUNTYP=ENERGY
  CCTYP=CR-CC
$END

$CONTRL
  RUNTYP=OPTIMIZE
  CCTYP=CCSD(T)
$END

CR-CCSD(T) energy calculation

CCSD(T) geometry optimization
More `$CONTRL` options

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>ICHARG</td>
<td>Charge on the system</td>
</tr>
<tr>
<td>MULT</td>
<td>Multiplicity</td>
</tr>
<tr>
<td>UNITS</td>
<td>Units to use (A, au)</td>
</tr>
<tr>
<td>MPLEVL</td>
<td>Order for Perturbation Theory</td>
</tr>
</tbody>
</table>
$SCF$

$SCF$

DIRSCF= TRUE.

$END$

Chooses a direct SCF algorithm where 2-e integrals are not stored to disk.
Change SCF convergence criteria (Δdensity < 10^{-6})
The $GUESS$ group controls the initial guess for the wavefunction. The wavefunction can start with guesses like the Huckel guess, or a guess can be read in.
$VEC

$GUESS  GUESS=MOREAD  $END

$VEC
1  1.90298197E-02  1.57336398E-02  6.36624695E-05  1.45119939E-05  5.71004537E-05
1  2  2.61483960E-04  1.54780421E-04  3.10647565E-06  1.70247089E-04  -5.17779168E-04
1  3  -1.60678663E-04  2.37314172E-04  -6.72251237E-05  2.12209422E-04  -8.71898945E-05
...
$END

Allows you to restart a SCF procedure, or use a known good starting guess for the orbitals.
$CIDET$

- $CIDET$
  - NCORE = 0
  - NACT = 22
  - NELS = 8
$END$

Used for FCI and MCSCF wavefunctions
$\text{CIDET}$

- $\text{CIDET}$
  - NCORE = 0
  - NACT = 22
  - NELS = 8
  - $\text{END}$

Number of doubly occupied Core orbitals

Number of active orbitals

Number of active electrons
Resource Considerations

- Should I run the job in parallel?

- How much memory do I need?
This group sets time limits and memory usage

SYSTEM group

SYSTEM
MEMORY=128000000
MEMDDI=100
TIMLIM=60 ← This job will terminate in 60 minutes

$END
$SYSTEM group

$SYSTEM
MEMORY=1280000000
MEMDDI=100
TIMLIM=60
$END

- MEMORY is the replicated memory used on each processor (in 8-byte words)
MWORDS is an alternative to the MEMORY keyword. It is the replicated memory used on each processor (in units of 1,000,000 8-byte words).
$SYSTEM
MWORDS=128
MEMDDI=100
$END

- MEMDDI is the total memory used for distributed data in units of 1000000 words
Memory Usage

If you run GAMESS on a single node, the total memory used will be:

\[(\text{MEMDDI} + \text{MWORDS} \times \text{NPROC}) \times 8 \text{ MB}\]

For each node when run on multiple nodes:

\[(\text{MEMDDI} + \text{MWORDS} \times \text{NPROC}) \times 8 \text{ MB} / \text{NNODES}\]

\text{NPROC} = \text{total number of processors used}
# Parallel Capabilities

<table>
<thead>
<tr>
<th>SCFTYP</th>
<th>RHF</th>
<th>ROHF</th>
<th>UHF</th>
<th>GVB</th>
<th>MCSCF</th>
</tr>
</thead>
<tbody>
<tr>
<td>Energy</td>
<td>P</td>
<td>P</td>
<td>P</td>
<td>P</td>
<td>P</td>
</tr>
<tr>
<td>analytic gradient</td>
<td>P</td>
<td>P</td>
<td>P</td>
<td>P</td>
<td>P</td>
</tr>
<tr>
<td>numerical Hessian</td>
<td>P</td>
<td>P</td>
<td>P</td>
<td>P</td>
<td>P</td>
</tr>
<tr>
<td>analytic Hessian</td>
<td>P</td>
<td>P</td>
<td>-</td>
<td>P</td>
<td>P</td>
</tr>
<tr>
<td>MP2 energy</td>
<td>P</td>
<td>P</td>
<td>P</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>MP2 gradient</td>
<td>P</td>
<td>P</td>
<td>P</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>CI energy</td>
<td>P</td>
<td>P</td>
<td>-</td>
<td>P</td>
<td>P</td>
</tr>
<tr>
<td>CI gradient</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>CC energy</td>
<td>P</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>EOM energy</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>DFT energy</td>
<td>P</td>
<td>P</td>
<td>P</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>DFT gradient</td>
<td>P</td>
<td>P</td>
<td>P</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>
How many processors should I use?

At least 4 for all methods that are parallelized.

Up to 64 processors for HF, DFT, and CI energies
How do I specify the calculation should be run in parallel?

This is handled by the rungms script that comes with GAMESS. When you submit calculations at MSI, this can be handled through the qgms script, e.g;

```
qgms -m 300mb -p 2 myinput.inp
```
Memory management

- READ the OUTPUT!

- GAMESS will tell you how much memory it’s using, and it will notify you what decisions it’s making based on the amount of memory you gave it.
GAMESSPLUS

- A plug-in for GAMESS to add solvation calculations and additional DFT methods.
If this group is present in your input file, GAMESS or GAMESSPLUS will run a DFT calculation

$DFT$DFTTYP=MPW1K  NRAD=80  
NTHE=16  NPHI=32 $END$
There are several functionals available in GAMESS

- MPW1PW91, MPW1K, and others have been added in GAMESSPLUS
New $groups for GAMESSPLUS input

$GMSOL or $CM2

- **ISCRF=0**: gas-phase Löwdin, RLPA, CM2, CM3, or CM4 charges
- **ISCRF=1**: solution-phase Löwdin, RLPA, CM2, CM3, or CM4 charges
- **ISCRF=2**
New $groups for GAMESSPLUS input

$GMSOL or $CM2

ISCRF=1

solution-phase charges with non-diffuse basis sets

ISCRF=2

solution-phase charges with diffuse basis sets
$GMSOL$

ICMD=319
Set of coefficients to used for CMX charges

ICDS=319
Set of coefficients to used for atomic surface tension parameters
Solvation calculations

- Check the GAMESSPLUS manual and associated publications for proper use of solvation methods.

- Certain solvation methods are designed to work well with certain basis sets.
Create Input File

- vi (all machines)
- pico (all machines)
- Molden (regatta, SDVL Linux and IRIX)
- Gaussview 😊
Running jobs interactively at MSI

module load gamess
rgms myinput.dat

module load gamessplus
rgmsp mygmspinput.dat
Running jobs interactively at MSI

module load gamessplus
rgmsp
qgmsp –p 2 –m 400mb

module load gamessplus
rgmsp
Running jobs interactively at MSI

module load gamessplus
rgmsp
qgmsp -p 2 -m 400mb

module load gamessplus
rgmsp
Submitting jobs at MSI

`qgmsp -p 2 -m 400mb`

memory requested is total memory (not memory/processor)
Output

• Make sure to read the output

GAMESS will print out more information by default as compared to other electronic structure codes.

Read the output from a couple calculations to see all the useful feedback on what GAMESS thinks of your input options.
Visualization

- Molden (regatta)
- Jmol (any platform, see: jmol.sourceforge.net)
Molden
J Mol
Questions?

GAMESS: www.msg.ameslab.gov/GAMESS

GAMESSPLUS:
comp.chem.umn.edu/gamessplus

Please send tutorial suggestions and questions to:

email: help@msi.umn.edu