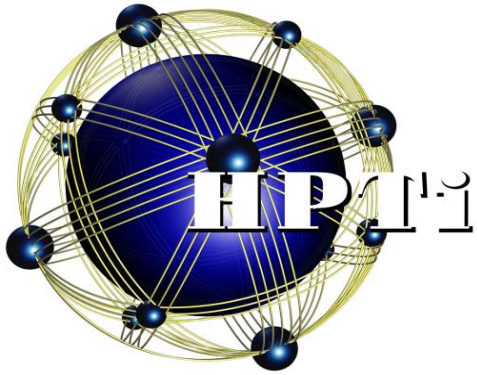

Using ACES II and ACES III

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presented at the DoD HPCMP UGC'06

What is ACES?

- Advanced Concepts in Electronic Structure computational chemistry package
- *ab initio* correlated wavefunctions from single-determinant reference wavefunctions in Gaussian basis sets
- single-point properties, geometry optimizations, point-group symmetry
- ground, excited, ionized, and attached states

ACES Program Suite

- ACES II
  - **`xaces2`** driver
  - **`xjoda`** brainstem
  - only serial binaries
- WinACES GUI
  - Python/Tkinter/Pmw (Windows and Unix)
  - creates input files
  - runs, controls ACES II
- pACES II
  - **`xp_aces2`** driver
  - **`xgemini`** remote mgr
  - “parallel” ACES II but only for numerical derivatives
- ACES III
  - **`xaces3`** parallel driver
  - SCF, MBPT(2), CCSD energies and gradients

ACES II - Environment

- **`xaces2`** uses **`system()`** to run programs
  - directory of binaries must be in login **`PATH`**
- most MSRC and some DC machines
  - sh (add to **`~/.profile`**):

```
. ~yau/arch/profile
```

  - csh (add to **`~/.cshrc`**):

```
source ~yau/arch/cshrc
```

- resource files set **`ACES_PATH`** and prepend to **`PATH`**

ACES II - Input Files

- **ZMAT**
  - sole input for molecule and keywords
  - Internal or Cartesian geometries
- **GENBAS**
  - basis set library
  - most from EMSL, some custom
- **ECPDATA**
  - effective core potentials (like **GENBAS**)

ZMAT - Header (optional)

- vertical blank space (spaces and tabs)
- comments (first non-blank char is **#**)
- file directives (first non-blank char is **%**)
  - directives redirect most file locations

    % GENBAS = /home/yau/Basis/GENBAS
  - special **SAVEDIR** directive is for restarts

    % SAVEDIR = /home/whoami/job1.save

ZMAT - Molecule Definition

- one-line title (required)
  - first non-blank, non-comment, non-directive line
- Z-matrix or XYZ matrix
  - trailing comments with #
  - no vertical gaps (i.e., comments or blank lines)
- Z-matrix parameters
  - one blank line separates Z-matrix from internal coordinate parameters

ZMAT - Namelists

- ***ACES2** is the primary list of keywords
  - case-insensitive except for names of basis sets
- ***VSCF** and ***INTGRT** are for DFT calcs
  - only used if ***ACES2(SCF_TYPE=KS)**
- ***GAMESS** controls GAMESS direct integrals
  - only used if ***ACES2(INTEGRALS=GAMESS)**
- ***SIP** controls ACES III options
  - pseudo-programming with **SIAL_PROGRAM**

ZMAT - Example (Internals)

```
# not the title you are looking for

a fine water calculation (the title)
H
O 1 R
H 2 R 1 A

R=1.0
A=109.5

*ACES2(calc=ccsd,basis=DZP)
```

ZMAT - Example (Cartesians)

```
% SAVEDIR = /home/yau/a2save

an optimization of XYZs
H -1.0  0.0 -1.0
O  0.0  0.0  0.0
H  1.0  0.0 -1.0

*ACES2(calc=mbpt(2),basis=DZP
geom_opt=full)
```

ACES II - Typical Run

```
> ls
   ZMAT     GENBAS
> xaces2 > out
> ls
   AOBASMOS  GENBAS  IIII  JOBARC   JAINDX
   MOL       NEWMOS  ZMAT  ZMAT.BAS out     …
> more out
   ************************************************
   * ACES : Advanced Concepts in Electronic Structure *
   *                 based on v.2.6.0-RC2             *
   *                 exported 17 JUN 2006             *
   ************************************************

   …
```

ACES II - Finding Data

- grep for energies

```
'E(SCF)='
'Total MBPT(2) energy'
'CCSD *energy is'
'CCSD(T) *='
```

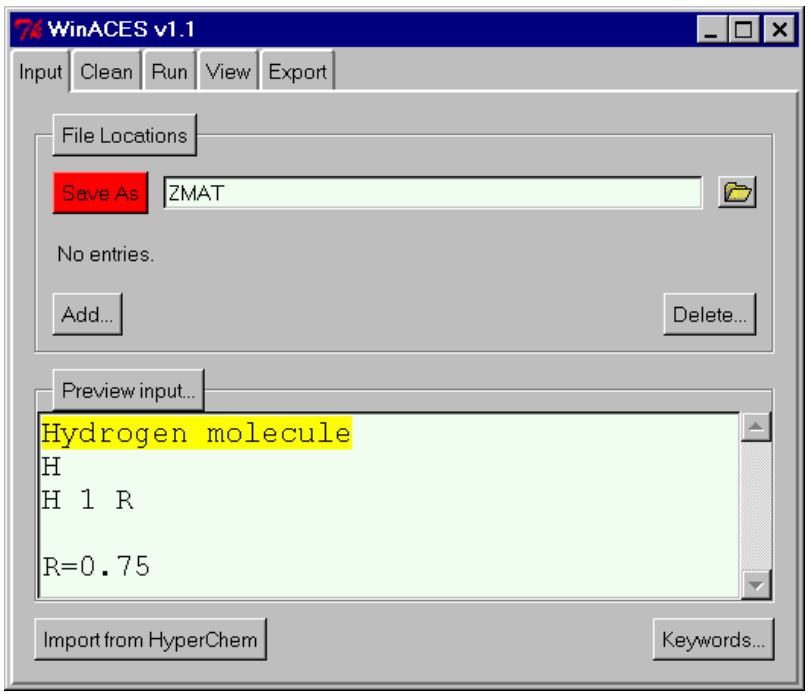
- sed for geometries and frequencies (end of file)

```
'/Summary of optim/,/convergence/p'
'/force constants/,/Zero-point/p'
```

Questions on running ACES II

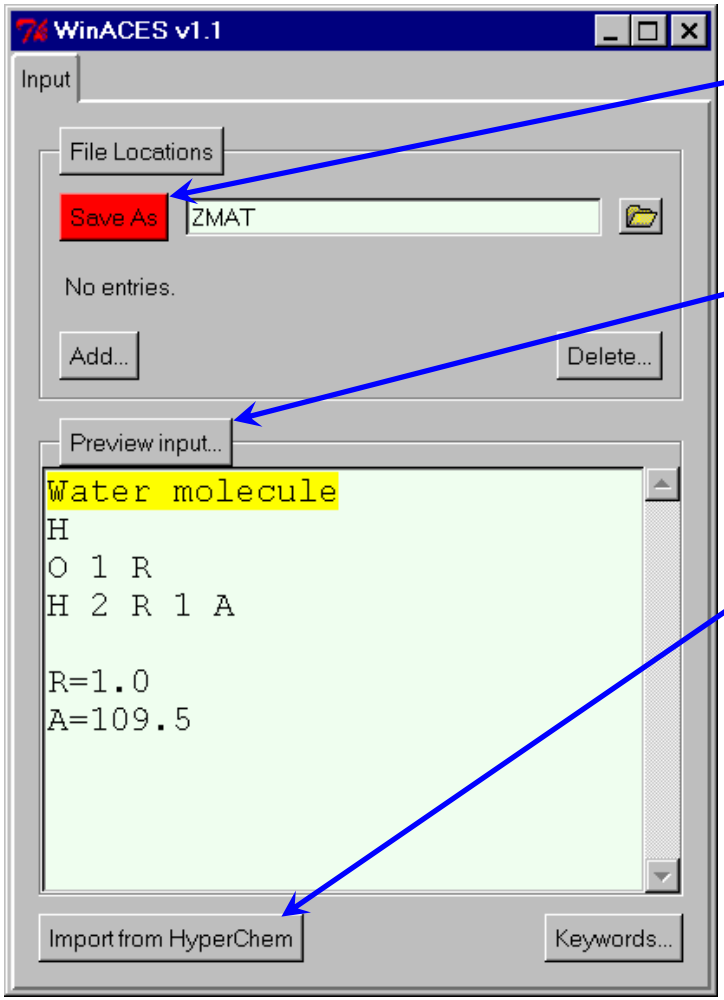
???

WinACES GUI



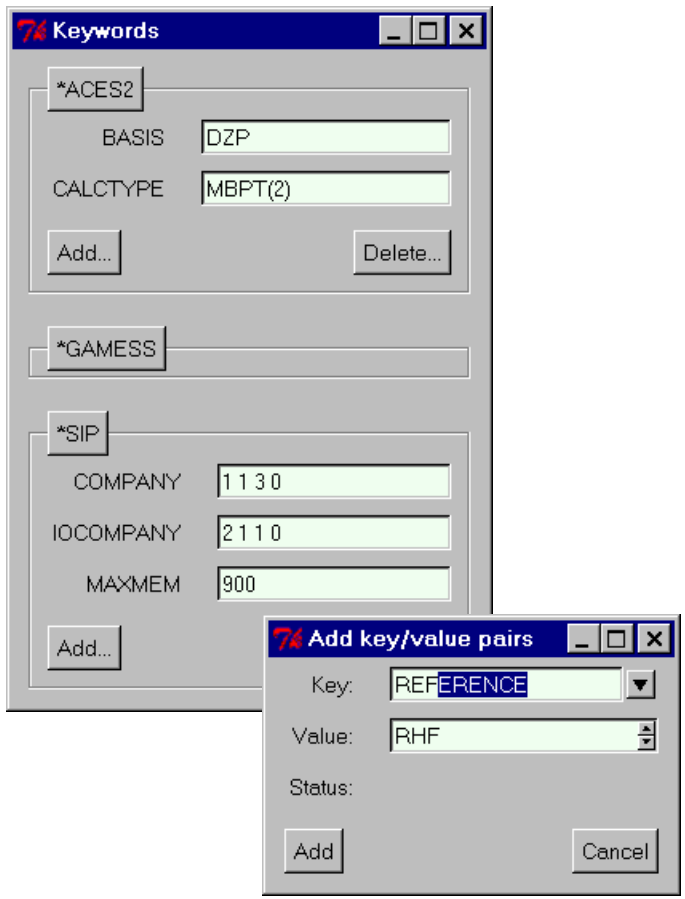
- Input file editor
- Windows:
  - import from HyperChem
  - cannot run ACES II
- Unix version:
  - no HyperChem
  - can run serial ACES II
- both versions require:
  - Python, Tkinter, Pmw

WinACES - input tab



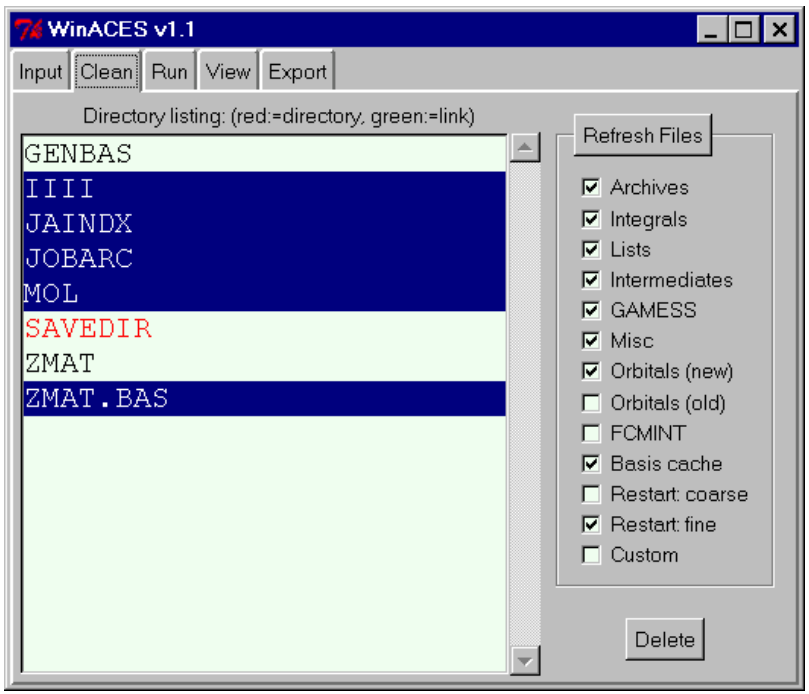
- Visual cue that file needs to be saved
- Preview button displays full ZMAT file for cut-n-paste
- MS Windows can import from HyperChem

WinACES - keyword menus



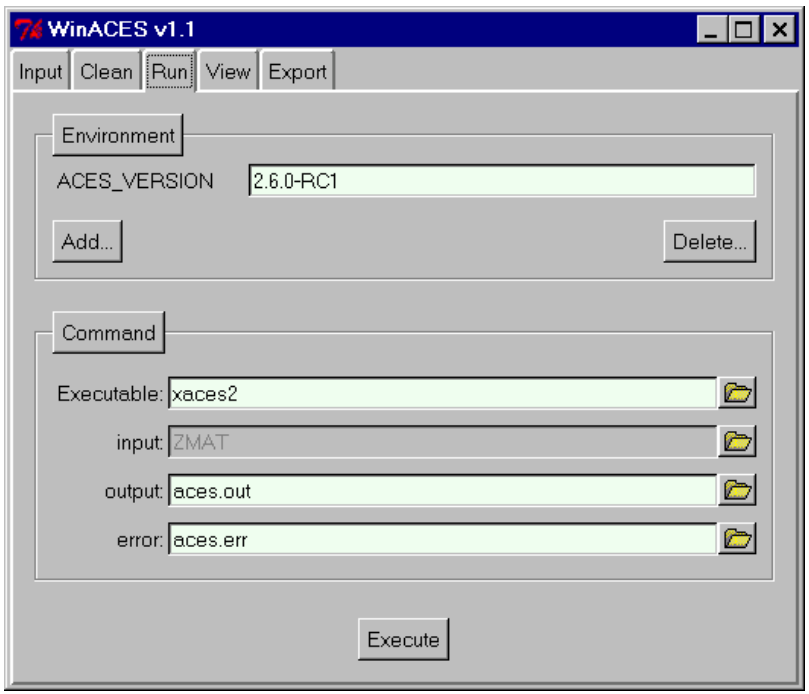
- Add known keywords to various namelists
- Suggest-as-you-type in the keyword field
- Select accepted values from a list
- Status field offers guidance (like units)

WinACES - clean tab



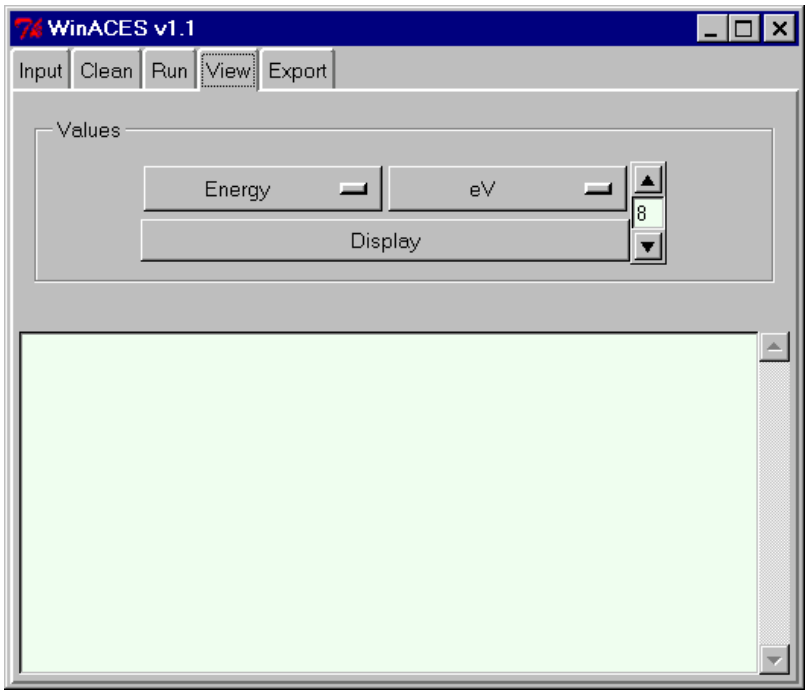
- Unix version only
- Pre-defined file sets allow users to safely delete program files
- Refresh button allows WinACES to respond to a background ACES job

WinACES - run tab



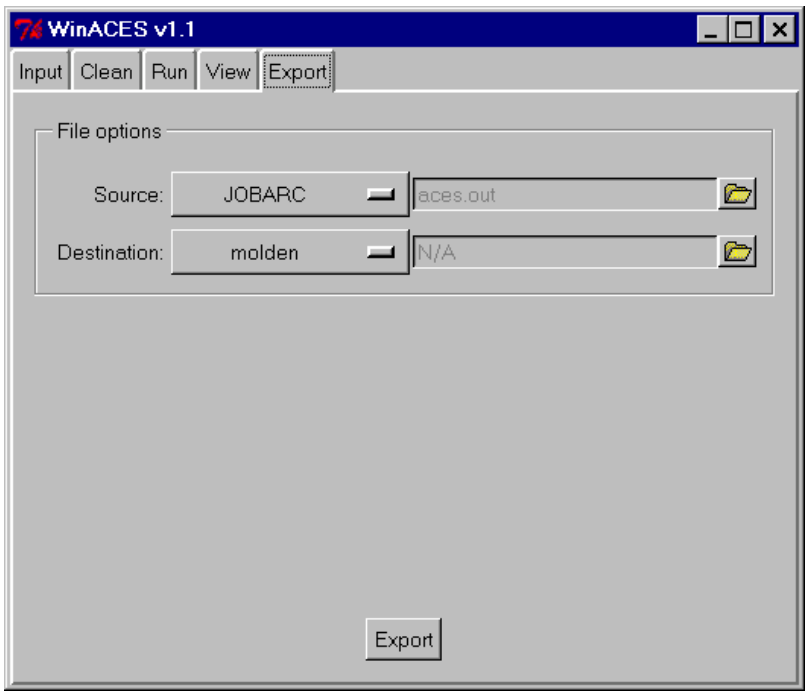
- Unix version only
- Set environment variables
- Set the executable
- Set output and error files

WinACES - view tab



- Unix version only
- Peek at values from the program
- Change units in real-time
- Change the number of decimal digits in real-time

WinACES - export tab



- Unix version only
- Export program data to other formats
- Currently limited to Molden and HyperChem, but the sky is the limit!

Questions on WinACES

???

pACES II - Overview

- Numerical first and second derivatives calculate values over a grid of nuclear displacements.
- **`xp_aces2`** runs just like **`xaces2`** but distributes the grid of displacements over all of the parallel tasks.
- pACES II applies to *all* ACES II methods.

pACES II - Why not?

- Every parallel task carries the full weight of a serial ACES II calculation – I/O and all!
- Very coarse-grain parallelization has load-balancing and scalability issues.
  - highest theoretical speedup equals the number of displacements
- Files in temp directories could be scattered all over the place. (Although this is sometimes a strength.)

Gemini - Directory Mgmt

- **`xgemini`** creates and destroys a private work directory for each parallel task
- a rich set of naming macros give fine control over where the directories are created
  `/usr/var/tmp/@LOGNAME@/job.@RANK@`
- **`xgemini`** can run serial programs in each directory

pACES II - Typical Run

```
> ls
   ZMAT     GENBAS
> run -tagio xgemini -s -i
> run -tagio xp_aces2 > out
> run -tagio xgemini -s -x
> seppoe out # separate lines of output
> ls
   ZMAT     GENBAS      out   out.0        out.00
   out.1    out.2       …
```

Questions on running pACES II

???

ACES III - Environment

- **`xaces3`** uses **`system()`** to run **`xjoda`**
  - directory of binaries must be in login **`PATH`**
- use resource files in **`~yau/arch`**
- resource files set **`ACES_EXE_PATH`** and prepend to **`PATH`** (if different from **`ACES_PATH`**)

*SIP Namelist - Companies

COMPANY = 1 1 W 0

W sets the number of compute tasks (workers).

IOCOMPANY = 2 1 M 0

M sets the number of storage tasks (managers).

- Guidance:
  - Total MPI tasks should equal **W+M** (about 7 workers to 1 manager).
  - Always set the other three integers as shown.

*SIP Namelist - SIAL programs

- multiple occurrences act like a script

```
SIAL_PROGRAM=scf_uhf_isymm_diis10.sio
SIAL_PROGRAM=tran_uhf_ao_dist1.sio
SIAL_PROGRAM=ccsd_uhf_ao_dist1_diis5.sio
```

- formalism will be replaced with macros or will be deduced from ***ACES2** settings
- Guidance:
  - maintain a list of scripts for reuse
  - **$ACES_EXE_PATH/sio** contains the sio files

***SIP** Namelist - segments

- **SIP_MX_OCC_SEGSIZE, SIP_MX_VIRT_SEGSIZE**
- segments define the largest range of array indices to be processed in one instruction
- **xaces3** tries to set these automatically
- Guidance:
  - small segments overflow the message buffers
  - large segments exhaust local memory
  - let **xaces3** set the values and only override if they cause problems

ACES III - Finding Data

- SIP has no knowledge of variable “names”
- grep for **`'Total energy:'`**
- geometries and frequencies printed the same as ACES II

Troubleshooting

- program not found
  - ensure **`xjoda`** is in **`PATH`** at the initial prompt
- basis set not found
  - remove **`ZMAT.BAS`** and check **`GENBAS`**
- **`xacesn`** just hangs
  - ensure **`COMPANY`** and **`IOCOMPANY`** have a 1 and 2 in the first integer values, respectively
- “blocks do not exist” error
  - try resubmitting with 1 or 2 more managers

Troubleshooting (cont.)

- (more)

Questions on running ACES III

???

Other Sources

- **http://www.qtp.ufl.edu/Aces2**
  - main ACES II web site with manuals and scripts for downloading
- **http://crisp.qtp.ufl.edu**
  - ACES III project server
- **yau@qtp.ufl.edu** or
- **anthony.yau@arl.army.mil**

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  - GSA Task Order No. 4THZ97064503
- US Army Research Laboratory
- University of Florida

Part 2: Hands-on exercises

(after quick break)

LSF	PBS	LL	GE
-P proj			-P
-q name			-pe
-n #			
-m jvn			
-a resrc			-l resrc
-W hh:mm			
			-S shell