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@ the University of Utah

Computational Chemistry Packages at CHPC

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http://www.chpc.utah.edu

Purpose of Presentation

- **Identify the computational chemistry software and related tools currently available at CHPC**
- **General overview of package capabilities**
- **Next talk : April 24, 2008**
  - **Focus on use of Gaussian03 and Gaussview at CHPC**

Arches Metacluster

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marchingmen.chpc.utah.edu (MM)

- 179 dual processor nodes
- 2GB memory/node
- /scratch/serial, /scratch/mm, /scratch/serial-old; local scratch (/tmp)
- 72 hr walltime maximum

tunnelarch.chpc.utah.edu (TA)

- 63 dual processor nodes
- 4GB memory/node
- /scratch/serial, /scratch/serial-old; local scratch (/tmp)
- 120 hr walltime maximum
- Can get increase of max walltime if needed

delicatearch.chpc.utah.edu (DA)

- 256 dual processor nodes
- 2GB memory/node
- /scratch/serial, /scratch/da, /scratch/serial-old; local scratch (/tmp)
- 72 hr walltime maximum - NEW

sanddunearch.chpc.utah.edu (SDA)

- 156 quad processor nodes
- 8GB memory/node
- /scratch/serial, /scratch/serial-old; local scratch (/tmp)
- 72 hr walltime maximum

landscapearch.chpc.utah.edu (LA)

- PI-Owned nodes of differing types (dual and quad) and amounts of memory
- Must belong to owner group to use
- One CHPC owned node – quad with 32GB memory, request access if needed

Batch

- **All use of compute nodes go through a batch system using Torque (PBS) and Maui (Moab) for scheduling**

```
#PBS -S /bin/csh
#PBS –l walltime=24:00:00,nodes=1:ppn=2
#PBS -N test
```

- **Login nodes only for prepping input files, analyzing results, compilations, etc – no running of jobs**

Arches scratch

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- **Details on scratch systems available**
  - **Local (/tmp) is about 30gb on most of arches; higher on SDA (60gb) and varies among LA nodes**
  - **/scratch/serial-old; /scratch/mm; /scratch/da - nfs**
    - **Each about 1.1 TB**
  - **/scratch/serial – nfs – NEW – 16.5 TB**
  - **/scratch/parallel will be gone in the next month or two**
- **Scratch space should not be used for storage of important files – the space is not backed up!**
- **CHPC reserves the right to scrub files older than 14 days as needed**
- **CHPC currently scrubbing files untouched for 60 days on a weekly basis**
- **Users need to be diligent about cleaning up after jobs**
  - **especially jobs that run out of time or do not finish properly!**

Security Policies

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- You may No clear text passwords - use ssh and scp
- Do not share your account under any circumstances
- Don't leave your terminal unattended while logged into your account
- Do not introduce classified or sensitive work onto CHPC systems
- Use a good password and protect it

Security Policies

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- **Do not try to break passwords, tamper with files, look into anyone else's directory, etc. – your privileges do not extend beyond your own directory**
- **Do not distribute or copy privileged data or software**
- **Report suspicions to CHPC (security@chpc.utah.edu)**
- **Please see http://www.chpc.utah.edu/docs/policies/security.html for more details**

Username/Password

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- CHPC has moved to the use of unids (UU ID number with first 0 replaced by u) and associated password
- Authentication/password maintenance done on campus level
- See nid.utah.edu for more information on setting/changing passwords

Access to CHPC Systems

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- **From Windows machine:**
  - **Need ssh client (recommend PuTTY)**
    - **http://www.chiark.greenend.org.uk/~sgtatham/putty/**
  - **For Xwindowing – need tool to display for Gaussview and ECCE**
    - **XLiveCD**
      - **http://xlivecd.indiana.edu/**
    - **Exceed (need 3D) available through OSL (www.osl.utah.edu) for about $100**
    - **XWin32 – free through OSL**

Default login script

- CHPC maintains default login scripts that will set up necessary environment for batch commands and many of the programs to work
  - http://www.chpc.utah.edu/docs/manuals/getting_started/code/chpc.tcshrc
  - http://www.chpc.utah.edu/docs/manuals/getting_started/code/chpc.bashrc
- Copy and put in your home directory as .tcshrc or .bashrc
  - This is being done on new accounts
- Can comment out setups for packages not used
- Default ones provided have chemistry package setups commented out – need to remove # at start of line
- Can customize by creating .aliases file that is sourced at end of the CHPC script

Current Computational Chemistry Packages...

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- Gaussian03
- NWChem
- GAMESS
- Amber
- Molpro – serial only
- Dalton – serial only

- There are several other packages that CHPC has experience installing, but that have to be licensed on a research group basis
  - Charmm
  - VASP
  - Crystal (98 version)

- Most installations are in /uufs/arches/sys/pkg/

...And Other Useful Tools

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- **On arches:**
  - Gaussview
  - Molden
  - Babel (Openbabel)
  - Dock and AutoDock (relatively untested)
  - Cambridge Structural Database
- **Others:**
  - ECCE
    - access from carbon.chpc.utah.edu

General Information

- **Available on CHPC web pages**
  - **Can get to from www.chpc.utah.edu -> Docs -> Software http://www.chpc.utah.edu/docs/manuals/software**
  - **Available for most packages**
  - **Has information on licensing restrictions, example batch scripts, where to get more information on a specific package**
  - **Also has useful information on running of jobs (scaling, issues, etc)**

OpenBabel

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- **Tool to interconvert structure files between a number of formats used in molecular modeling**
- **To run:**
  - **source /uufs/arches/sys/openbabel/etc/babel.csh (or uncomment in your tcsh)**
  - **babel -i < input-type > < infile > -o < output-type > < outfile >**
  - **babel –H to see format for usage, options, and input/output file-types**

GaussView

- Molecular builder and viewer for Gaussian input/output files
- Have version 4 (std) on arches
  - Have campus licenses for linux version
- Still have old GaussView 3.09 for windows
- Access with "gv&" – provided you have uncommented the Gaussian setup from the standard .tcshrc
- DO NOT submit jobs from within GaussView – instead create and save input file and use batch

ECCE

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- **Extensible Computational Chemistry Environment – current version 4.5.1; CHPC has 4.0.1 installed**
- **Package developed at EMSL at PNNL**
- **Set of modules to manage computational chemistry computer jobs (Gaussian03, NWChem) from start to finish all from your desktop system**
- **Installed on carbon.chpc.utah.edu**
- **User accounts need setup – see me if interested**
  - **carbon is not always kept running**

Within ECCE you can..

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- Build molecules/import structures
- Create input files for jobs using pull down menus of possible options
- Look at what resources available on different computer systems
- Launch jobs on any of these resources and then monitor job progress/view output
- Store/organize results in personal database
- Needs Xwindowing software if using from a PC

- If there is interest, I can schedule a separate demonstration on ECCE & its capabilities or user can schedule an appointment for a demo

Molden

- Another program for viewing molecular/ electronic structures
- Works with Gamess, Gaussian, Molpro
- Supports plots of Electronic density, MOs, etc
- More information at http://www.cmbi.ru.nl/molden/molden.html
- How to use at CHPC:
  - Make sure your path includes /uufs/arches/sys/pkg/molden
  - Molden4.6 &

Dock

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- Programs to look at binding of a small molecule within the active site of a receptor, usually a macromolecule
- Version 6.1installed (6.2 available)
- Get info at: http://dock.compbio.ucsf.edu
- Available on all of arches at /uufs/arches/sys/pkg/dock/std/bin/
- To run
  - source /uufs/arches/sys/pkg/dock/etc/dock.csh
  - dock6.mpi to start (needs arguments)

Autodock

- Also docks ligands (flexible) to macromolecular receptors
- http://autodock.scripps.edu
- We have version 3
  - Will update to version 4 in near future
- Will look at possibility of installing the AutoDockTools for graphical interface
- Available on all of arches at /uufs/arches/sys/pkg/autodock/std
- To run:
  - source /uufs/arches/sys/pkg/autodock/etc/autodock.csh
  - autodock3

Cambridge Structural Database

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- Moved from library to CHPC summer 2006
- www.ccdc.cam.ac.uk for information
- Need CHPC account to use
- Need to have PC with Xterm/Xwindowing software (Putty/XLiveCD work well) to start session on any of arches interactive nodes
  - source /uufs/arches/sys/pkg/CSD/std/cambridge/etc/csd.csh
  - cq & <- to start conquest (search engine)
  - mercury & <- to start crystal structure viewer
  - The first time you use it will ask you to confirm licensing
    - need to provide site/license codes (840/097537)first time

Amber

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- **Molecular mechanics/dynamics package with associated force field**
- **Current version is Amber9 (Amber10 just ordered)**
- **Basic information on getting started on arches: http://www.chpc.utah.edu/docs/manuals/software/amber.html**
- **For further assistance**
  - **the Amber email reflector is very useful**
  - **Can also contact Tom Cheatham (Amber developer) at cheatham@chpc.utah.edu**
- **For more information see http://amber.scripps.edu**

Amber – getting started

- **setenv AMBERHOME appropriately:**
  - **SERIAL: /uufs/arches/sys/pkg/amber/amber9/opteron-pathscale-serial-static/exe**
  - **PARALLEL, DA with myrinet: /uufs/arches/sys/pkg/amber/amber9/opteron-pathscale-mpich-mx/exe**
  - **PARALLEL, SDA with infiniband: /uufs/arches/sys/pkg/amber/amber9/opteron-pathscale-mpich-mvapich/exe**
  - **PARALLEL, TA and MM: /uufs/arches/sys/pkg/amber/amber9/opteron-pathscale-mpich/exe**
- **set path = ($path $AMBERHOME/exe)**
- **sander**
  - **Program in amber that does actual energy minimization; parallel version (mpi) exists**
  - **Example scripts on chpc web page**
- **antechamber and xleap**
  - **Interactive programs in amber to help create input files (find with serial build)**
- **New ambertools package now available**

Molpro

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- Program emphasis is on highly accurate computations, with extensive treatment of the electron correlation through multi-configuration reference CI, coupled cluster and associated methods
- For more information http://www.molpro.net
- Current version 2006.1; only serial operation available
- Installed on arches:
  - /uufs/arches/sys/pkg/molpro/std-serial/bin
- Sample script available on molpro on chpc software pages
  - http://www.chpc.utah.edu/docs/manuals/software/molpro.html

Dalton

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- Focus on property calculations at HF, DFT, MCSCF and CC levels of theory
- I have sample input files for NMR shielding calculations
- Version 2.0 installed
- For more information:
  - http://www.kjemi.uio.no/software/dalton/dalton.html
- Only serial build available currently
- Location:
  - /uufs/arches/sys/dalton-serial/bin
- For information on accessing CHPC installation
  - http://www.chpc.utah.edu/docs/manuals/software/dalton.html

Gaussian03

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- **Commercial electronic structure package**
  - **http://www.gaussian.com for information and User's Guide**
- **Current installed revision of G03 is E.01 on arches**
  - **/uufs/arches/sys/g03**
  - **Has been updated to include latest NBO5**
- **For information on accessing the CHPC installation**
  - **http://www.chpc.utah.edu/docs/manuals/software/g03.html**

General Info on Arches

- To run G03 on arches you will need to have the .tcshrc file that CHPC provides in your home directory – even if you normally run a bash shell – as gaussian jobs run under a csh environment
- Users need to request to be put in the gaussian users group so that they have permission to access installation
- Exampe test files can be found in
  - /uufs/arches/sys/g03/g03/tests/com (input files)
  - /uufs/arches/sys/g03/g03/tests/ia64 (output files)
  - Great resource for examples of different functionalities

Batch Execution

- **Sample PBS scripts for Gaussian03 on all platforms are availaible on the Gaussian03 CHPC web pages**
  - **http://www.chpc.utah.edu/docs/manuals/software/g03.html**
- **More detailed info on use – next week's talk**

NWChem

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- Package developed at PNNL to work on massively parallel systems
- Goal: Computational chemistry solutions that are scaleable with respect to both chemical system size and MPP hardware size
- Has quantum mechanics, molecular mechanics/dynamics, and quantum molecular dynamics
- version 5.0 installed on arches (with Python)
  - /uufs/arches/sys/nwchem/bin/LINUX64

NWChem Web Pages

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http://www.emsl.pnl.gov/docs/nwchem/nwchem.html

The site is searchable and covers:

- Capabilities
- User's Manual and Programmer's Manual - searchable
- Support
- Tutorial
- Benchmarks
- Applications
- FAQ's
- Known Bugs
- Platforms
- Download

Also need to have…

- **To run:**
  - **source /uufs/arches/sys/nwchem/etc/nwchem.csh**
- **More inforation and example batch script at**
  - **http://www.chpc.utah.edu/docs/manuals/software/nwchem.html**

GAMESS

- General Atomic and Molecular Electronic Structure System
- Another option for most ab initio quantum calculations
- On 22 February 2006 version
- http://www.msg.ameslab.gov/GAMESS for information on usage and capabilities
- Can run both parallel or serial
- For information on accessing the CHPC installation see
  - http://www.chpc.utah.edu/docs/manuals/software/gamess.html

Finally.....

- **Let us know if there is some other package that does something that our current packages do not; we can look into the possibility of getting it.**
  - **Factors: cost, hardware/OS requirements, licensing issues**
- **Any questions – contact me**
  - **anita.orendt@utah.edu**
  - **Phone: 231-2762**
  - **Office: 422 INSCC**