Chemistry Packages at CHPC

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Purpose of Presentation

- Identify the computational chemistry software and related tools currently available at CHPC
- Present overview of these packages
- Present how to access packages on CHPC
- Next talk – focus on Gaussian and GaussView – 20 November 2008
Brief Overview CHPC Resources

• **Computational Clusters** - Arches
  • **Home directory** – NFS mounted on all clusters
    – `/uufs/chpc.utah.edu/common/home/<uNID>`
    – generally not backed up (there are exceptions)
  • **Scratch systems** – global to all HPC systems
    – `/scratch/serial` (16 TB)
    – `/scratch/serial-old, /scratch/da, /scratch/mm, /scratch/serial-pio`
    – files older than 60 days removed
  • **Applications** - `/uufs/arches/sys/pkg`
Getting Started at CHPC

- Account application
  - www.chpc.utah.edu/docs/forms/application.html
- Interactive nodes
  - Two per each cluster (cluster.chpc.utah.edu) with round-robin access to divide load
- CHPC environment scripts
  - www.chpc.utah.edu/docs/manuals/getting_started/codes/chpc.tcshrc
  - www.chpc.utah.edu/docs/manuals/getting_started/codes/chpc.bashrc
- Getting started guide
  - www.chpc.utah.edu/docs/manuals/getting_started
- Problem reporting system
  - http://jira.chpc.utah.edu or email to issues@chpc.utah.edu
Batch System

• 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

• Login nodes only for prepping input files, analyzing results, compilations, etc – no running of jobs – 15 min MAX

• Walltime limits in place – 72 hours (TA 120 hours)
Security Policies (1)

- 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 – see gate.acs.utah.edu for tips on good passwords
Security Policies (2)

• 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
Access to Interactive Nodes

• 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 scripts

- 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.tcshrc)
  - [http://www.chpc.utah.edu/docs/manuals/getting_started/code/chpc.bashrc](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
Location of Installations

• Currently we place most installations at:
  – /uufs/arches/sys/pkg
  – /uufs/cluster.arches/sys/pkg

• In the process of moving installations to a three layer system:
  – /uufs/chpc.utah.edu/sys/pkg
    • Accessible on clusters and INSCC/Meteo linux desktops
  – /uufs/arches/sys/pkg
    • Accessible on all clusters
  – /uufs/cluster.arches/sys/pkg
    • Single cluster access
General Information

• Available on CHPC web pages
  – Can get to from www.chpc.utah.edu -> Software documentation -> More (for complete list) 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) for some applications
Chemistry Packages

- Quantum Codes
- Molecular mechanics/dynamics
- Support Packages
  - visualization
  - docking
  - conversion of file formats
  - structure database
Quantum Packages

- Gaussian03
- NWChem
- GAMESS
- Molpro – serial only
- Dalton – serial only
- VASP (licensed by individual research group)
Molecular Mechanics/Dynamics

- Amber
- NWChem
- Gromacs
- Charmm (licensed by research group)
Support Packages

• On arches:
  – Gaussview
  – Molden
  – VMD
  – NBOView
  – Babel (Openbabel)
  – Dock and AutoDock (relatively untested)
  – Cambridge Structural Database

• Others:
  – ECCE
    • access from carbon.chpc.utah.edu (Talk to me first)
OpenBabel

• 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

11/13/2008  http://www.chpc.utah.edu  Slide 17
GaussView

- Molecular builder and viewer for Gaussian input/output files
- Have version 4 (std) on arches
  - Have campus licenses for linux version
- Still have campus license for 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
NBOView

• Package to view NBO orbitals
• For information see http://www.chem.wisc.edu/~nbo5/v_manual.htm
• How to use at CHPC:
  – Add to your path: /uufs/arches/sys/pkg/nbowview/nbowview1.1
  – nbowview
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 &
VMD

- Visualization, mainly for MM/MD
- Reads a number of different file formats
- Information at http://www.ks.uiuc.edu/Research/vmd
- Can either install on own desktop (windows/mac/linux versions available)
  or use arches installation /uufs/arches/sys/pkg/vmd/vmd-std/vmd
ECCE

- 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 (including building system) to finish all from your desktop system
- Installed on carbon.chpc.utah.edu
- User accounts need setup – see me if interested as carbon is not always kept running
Dock/AutoDock

• Programs to look at binding of a small molecule within the active site of a receptor, usually a macromolecule
• Dock
  – version 6.1 installed (6.2 available)
  – get info at: http://dock.compbio.ucsf.edu
  – source /uufs/arches/sys/pkg/dock/etc/dock.csh
  – dock6.mpi to start (needs arguments)

• Autodock
  – version 4 being installed
  – info available at http://autodock.scripps.edu
  – source /uufs/arches/sys/pkg/autodock/etc/autodock.csh
  – autodock3
Cambridge Structural Database

- Moved from library to CHPC summer 2006
- www.ccdc.cam.ac.uk for information
- Need CHPC account to use
- From PC need 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`
    - Uncomment line in `.tcshrc` to do this upon login
  - `cq &` <- to start conquest (search engine)
  - `mercury &` <- to start crystal structure viewer
  - The first time you use it on a given computer you will be asked to confirm licensing
    - need to provide site/license codes (840/097537)
• Molecular mechanics/dynamics package Current version is Amber9 (working on Amber10 installation)
• 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
• Different parallel builds available for DA (myrinet) and SDA (infiniband) as well as generic mpi (for TA and MM)
GROMACS

- Another option for molecular dynamics
- Version 3.3.3 installed
- See http://www.gromacs.org/ for help
- Installation at /uufs/arches/sys/pkg/gromacs/std
- Both serial and parallel for mdrun
- Sample scripts on chpc web site
  - http://www.chpc.utah.edu/docs/manuals/software/gromacs.html
CHARMM

• Another molecular mechanics package
• Package is licensed per research group and for a specific version
• If interested – get license and we can do installation such that only your group has access.
• See www.charmm.org for details
Molpro

- 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
- Version 2006.1; only serial operation available
- Installed on arches:
  - /uuufs/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

- 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](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/sample scripts
  - [http://www.chpc.utah.edu/docs/manuals/software/dalton.html](http://www.chpc.utah.edu/docs/manuals/software/dalton.html)
Gaussian03

- Commercial electronic structure package
  - [http://www.gaussian.com](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](http://www.chpc.utah.edu/docs/manuals/software/g03.html)
NWChem

- 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`
- To run:
  - `source /uufs/arches/sys/nwchem/etc/nwchem.csh`
  - must have `$HOME/pdir` directory if running parallel
- More information 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](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](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
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