Desktop-to-Grid Chemistry

Dr. Shawn Sendlinger
Department of Chemistry
North Carolina Central University

Reality Check

- Model all water molecules in one drop of H_2O
  - Initial conditions:
    - Must know coordinates of each atom
    - How many coordinates is this?

$$1drop\left(\frac{1mL}{20drop}\right)\left(\frac{1g}{1mL}\right)\left(\frac{1mol}{18g}\right)\times$$

$$\left(\frac{6\times10^{23}molec}{1mol}\right)\left(\frac{3atoms}{1molec}\right)\left(\frac{3coord.}{1atom}\right)\approx \underline{1.5\times10^{22}coord.}$$

Reality Check - continued

- Assume machine can read in coordinates at the maximum processor speed (3 GHz)
- Time to initialize atomic coordinates:

$$1.5\times10^{22}\,coord.\left(\frac{1s}{3\times10^{9}}\right)\left(\frac{1hr}{3600s}\right)\left(\frac{1d}{24hr}\right)\left(\frac{1yr}{365d}\right)\approx 160kyr$$

- Using fastest supercomputer (BlueGene/L) at 281teraflops; Time ≈ 1.7yr
- NCSA machine @100petaflops; T ≈ 1.7 days

Desktop Comp. Chemistry

- What can be done on a desktop?
  - Use WebMO as the tool
  - Look at water and some small clusters (Handout)
- Static, *small*, *gas phase* clusters are doable
  - PM3 gives decent bond distances
    - PM3 calc. time scales as N^2-N^4 (N= # or orbitals)
  - Higher level of theory (B3LYP/3-21G) calculation on water dimer took 87 seconds
    - Gives better energy values
    - DFT calc/ time scales as N^3

Molecular Dynamics

- What if we want to observe motion?
- Simple approaches:
  - Phase diagram of water
  - Autoionization
  - Geometry optimization, small cluster
- Use calculations (2D): Molecular Workbench
  - Hydrogen bonds in water
  - Ion-dipole forces
  - Dissolving salt in water
  - Hydrophobicity and hydrophilicity

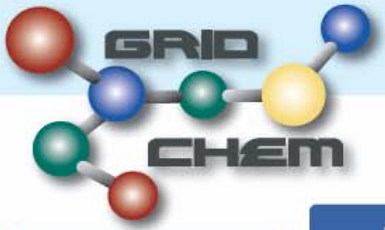
Molecular Dynamics - continued

- Can we do 3D on a desktop machine?
  - Odyssey Demo
    - Ice melting (Screen 3)
    - NaCl crystal (Screen 5)
    - Ion-dipole interaction (Screen 6)
    - NaCl dissolution (Screen 1)
    - Polar vs. nonpolar solutes (Screen 7)
    - Build your own? (Screen 8)
  - For a limited number of small molecules, we can do some molecular dynamics on a desktop

Beyond the Desktop

- Need more computational horsepower
  - More accurate calculations in reasonable time
  - Larger molecules
  - Molecular dynamics in biochemical systems
- Computational Chemistry Grid
  - Client application is **GridChem**
    - Java desktop application
      - Provides interface to integrate hardware, software, and middleware resources necessary to solve quantum chemistry problems using grid technologies

GridChem



Computational Chemistry Grid:

Production Cyberinfrastructure for Computational Chemistry

For more information, please visit www.gridchem.org or contact help@gridchem.org.

Computational Chemistry Grid (CCG)

- CCG is a 3-year, National Middleware Initiative (NMI) program to develop cyberinfrastructure for scientists engaged in studying molecular structure and function
- CCG allows scientists needing access to computational chemistry software to:
  - -Easily submit, monitor and manage jobs from a desktop client
  - -Access a large set of HPC systems and Chemistry software applications
  - -Streamline file transfer to/from HPC systems and the desktop client
- CCG integrates a desktop environment into an infrastructure for a broad community of users:
  - - Computational chemists with both small and large scale needs
  - - Experimentalists who need simulation capabilities to verify experimental results
  - - Scientists from disciplines outside of chemistry that need access to software for molecular simulations

CLIENT

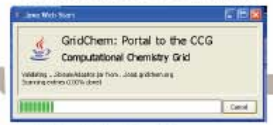
Graphical user Interface (GUI) :

- Interface for building and validating Gaussian and GAMESS input les
- Graphical view of CCG computational resources and system load
- Submit, monitor and manage jobs across all CCG resources from desktop client
- Integrated le transfer between CCG mass storage and desktop system

Client available for multiple platforms (Linux & Windows)

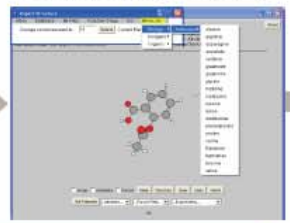
No Grid services needed on client system

JAVA WEB START



Client Application runs on Local Machine

BUILD MOLECULE



BUILD INPUT FILE

MONITOR CCG RESOURES

MANAGE JOBS

Middleware Server

Middleware interface to the computational grid

- authentication
- user, data, and job management
- real-time, user-centric grid monitoring
- cross-domain accounting
- incentive and predictive-based job scheduling
- pre- and post-execution data analysis
- long-term data storage
- multiple notification mechanisms

SUBMIT

FILES STAGED AUTOMATICALLY

Grid Services

Leveraging NMI Software

Dispatch Jobs To Resources

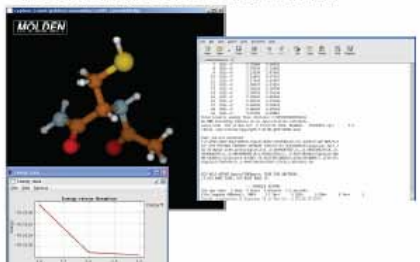
DOWNLOAD RESULTS

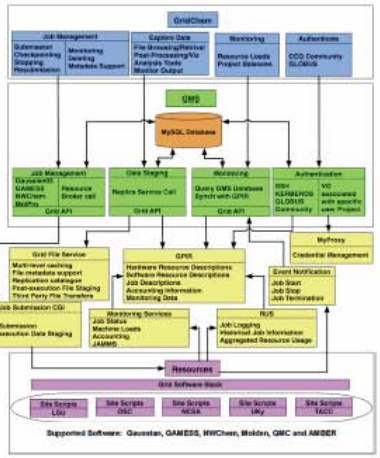
MONITOR OUTPUT (AUTOMATIC)

DOWNLOAD RESULTS

FILE BROWSER (MANUAL)

POST PROCESS REVIEW





Supported Software: Gaussian, GAMESS, NWChem, Molden, QMC and AMBER

CCG Resources

3,525,000 CPU hours available annually

Supported by the NSF NMI Program under Award #04-38312

NCSA www.ncsa.uiuc.edu

CCS Center for Computational Sciences UK University of Kentucky www.ccs.uky.edu

cct www.cct.lsu.edu

OSC www.osc.edu

TACC www.tacc.utexas.edu

Supercomputing

- Examples:
  - Ice melting
  - Octane and water
  - NaCl in octane
  - NaCl in water
  - NaCl in water (water not shown)
  - Water in a carbon nanotube
  - Micelle assembly of octanoate in pentane (pentane not shown)

Acknowledgements

- Robert Panoff
  - Shodor Education Foundation
- Scott Lathrop
  - SC07 Education Program Chair & TeraGrid Director of Education, Outreach and Training
- Clyde Metz
  - Professor Emeritus, College of Charleston
- Jay Mashl
  - Computational Chemists, UIUC