Computational Chemistry Grid (CCG)

- Goal: To Provide access to computational chemistry software, hardware and services using well established Grid technologies to a wide user community of expert, novice and non-traditional users.
- 3–year NSF NMI funded project Award #04-38312
- 5 partners:

OSC

NCSA

TACC

cct

CCS
Center for Computational Sciences

CCG Community Resources

System (Site)	Procs Available	Annual CPU hrs
OSC – Intel Itanium Cluster	580	380,000
TACC - IBM Power 4	16	40,000
NCSA – Platinum Condor Pool	64	
NCSA – (Copper) IBM Power4	384	20,000
NCSA – (Tungsten) Intel	2688	20,000
NCSA – SGI Origin 2000	128	1,000,000
NCSA - Intel Cluster	14	122,500
UKy – Intel Cluster	96	840,000
LSU – Intel Cluster	1024	1,000,000
Total	5026	3,322,500

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What CCG Does

- Existing computational chemistry resources are commonly accessed via a text interface and batch client.
- There is none of the ease of use of a desktop machine and the user must learn the system details of the remote machine
  - Queues
  - Number of nodes and processors
  - How to set time and memory limits
- CCG and the GridChem client allows the researcher to use these chemistry applications without having to learn these system details about one or more machines. This is done by having a Java desktop client that is the only part of the CCG that the researcher has to interface with.

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Supported Applications

- Gaussian03 (Currently the only one at OSC ipf cluster)
- GAMESS
- NWChem
- MolPro
- AMBER
- qmcPACK
- ACES-II**
- Columbus**
- Crystal**
- QChem**

**** Due in future release**

Software stack

- *Clusters*
  - *Globus 2.4*
    - *globus-gatekeeper*
    - *gsiftp*
  - *Gsissh/gsiscp*
  - *Uberftp client*
- *Server*
  - *Globus 4*
  - *Hibernate*
  - *Java 1.4+*
  - *Ant*
  - *Log4j – server side logging*
  - *JUnit – unit testing*
  - *Gsissh/gsiscp*
  - *Gridftp*
- *Client*
  - *Java 1.5 (webstart)*

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bcMPI: HPC Computational Science IDE on Itanium

Dave Hudak, Neil Ludban, Jaya Natarajan
Vijay Gadepally, Siddharth Samsi
Ashok Krishnamurthy

HPC Computational Science IDE (CSIDE)

- A suite of software tools, including
  - Numeric interpreter with high-level matrix operations
  - Domain-specific extensions (signal and image processing, control systems, operations research)
  - Graphics and visualization
  - Common user interface (usually including editor)
- Examples
  - Commercial: MATLAB, Maple, Mathematica
  - Open source
    - GNU Octave + OctaveForge + GNUPlot
    - NumPy + SciPy + iPython + Matplotlib
- Extending CSIDE to HPC system requires
  - Job control mechanism for launching a copy of interpreter on each processor
  - Communication libraries for interpreters to exchange results

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bcMPI - download version 1.1 on March 27, 2007

http://www.bluecollarcomputing.org

- Paramake - installer for bcMPI
  - UNIX tools, OpenMPI, bcMPI library, bcMPI toolbox, examples, GNU Octave (with vendor BLAS and fftw) if necessary
- bcMPI features
  - Runs on UNIX: tested on Linux, NetBSD, MacOS X
  - API “reasonably compatible” with MatlabMPI
    - bcMPI tags are numeric, MatlabMPI alphanumeric
  - Broadcast, barrier, reduce operations
  - bcMPI supports synchronous or asynchronous sends
    - MPI_Buffer_attach, MPI_Buffer_detatch, MPI_Probe
  - MPI communicator support (new in v1.1)
  - Supports many MATLAB data types, but no sparse support
  - MATLAB-style help for commands
- Integration with standard HPC environments and tools
  - Job control with PBS, LSF (new in v1.1)

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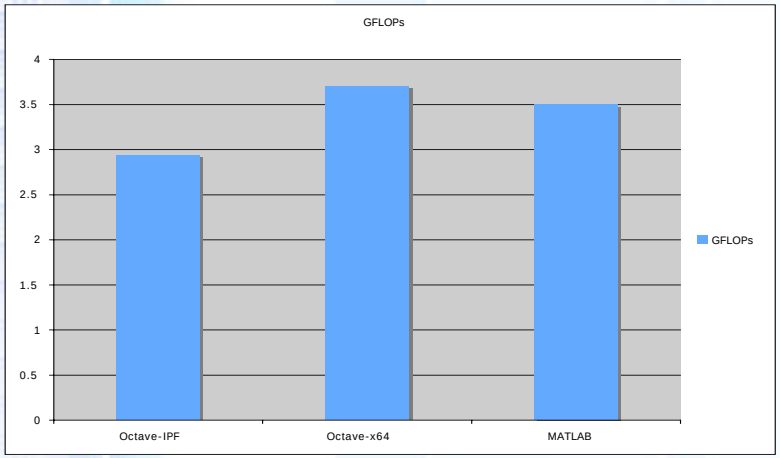
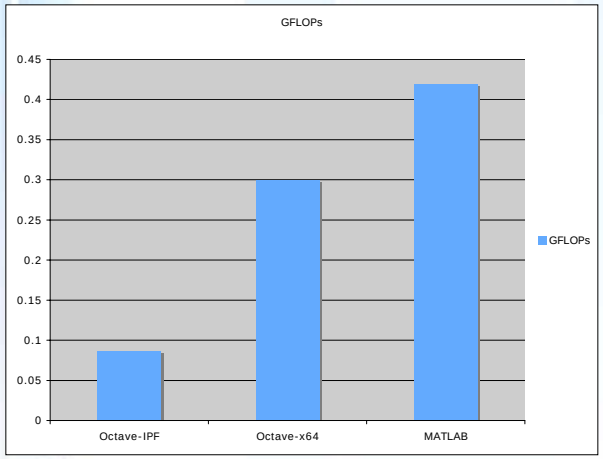
Intel MKL and FFTW use in Octave





- Octave v2.9.9. on 1.4 GHz Itanium 2
- Octave v2.9.9 on 2.4 GHz Opteron
- MATLAB R2007a on 2.4 GHz Opteron
- Top500 from HPC Challenge
- FFT from HPC Challenge

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NAS FT Results