Applications, Software and Supercomputing Environment in SCCAS

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Outline

- Brief Introduction of SCCAS
- Large Scale Applications
- Developed Software
- Supercomputing Environment
SCCAS-Computing Resources

- During 1996-2000 (9th 5 year plan)
  - In 1996, SGI Power Challenge XL
    - 6.4Gflops
    - 16 CPUs
  - In 1998: Hitachi SRR201
    - 9.6GFlops
    - 32CPUs
  - In 2000, Dawning 2000 II
    - 111.7Gflops
    - 164 CPUs
SCCAS-Computing Resources

- During 2001-2005 (10th 5 year plan)
  - In 2003, Lenovo DeepComp6800
    - 5Tflops, 1024 CPUs
    - TOP500: No.14; China TOP100: No.1

- During 2006-now (11th 5 year plan)
  - In 2008, Lenovo DeepComp7000
    - 150Tflops, 13,000 cores
    - TOP500: No.19; China TOP100: No.2
    - 3 kinds of nodes, Altix 4700, IBM 3950, IBM Blades
  - In 2009, 300TFLOPS GPU
SCCAS-Services: Users

- Users in SCCAS has massively increased since 1996 (from 20 to more than 320)
SCCAS-R&D of Algorithms and software

- Parallel AMR (Adaptive Mesh Refinement) method
- Parallel Eigenvalue Problem
- Parallel Fast Multipole Method
- Parallel Computing Model
- Gridmol
- ScGrid middleware
- PSEPS
- FMM-radar
- Transplant many open source software
Prediction of Sandstorm

- Real-time prediction system of Sandstorms in China Meteorological Bureau
- DeepComp6800
  - 256 CPUs
  - from 15 hours down to 8 mins
Global Climate Model-FGOALS

<table>
<thead>
<tr>
<th>CPU</th>
<th>AGCM</th>
<th>LAND</th>
<th>OGCM</th>
<th>ICE</th>
<th>Coupler</th>
</tr>
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<tbody>
<tr>
<td>1620</td>
<td>720</td>
<td>90</td>
<td>540</td>
<td>180</td>
<td>90</td>
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</tbody>
</table>
EM Scattering

- The surface currents and RCS of plane and destroyer models
  - Used for antenna design, RCS analysis
  - Stealth design of airplanes, etc.
Software Introduction

- Both are optimized InsPecT software
- P_InsPecT is open source and can be downloaded from SCBG
- Cuda-InsPecT will be open source

Software Function

- InsPecT is an unrestricted identification software of PTMs (post-translational modifications)

Software Characteristics

- **P_InsPecT**
  - via MPI
  - run on CPU cluster or CPU nodes of HPC

- **cuda-InsPecT**
  - via MPI+cuda C
  - run on GPU cluster

Software Performance

**Software**: P_InsPecT (one modification)
- **Database**: 36547 mass spectrometric; 107962 protein sequences
- **Environment**: DeepComp7000
  - **One Core**
    - **Time**: estimate 1177.7 h
  - **2048 Cores**
    - **Time**: 0.4 h

**Software**: cuda-InsPecT (two modifications)
- **Database**: 62346 mass spectrometric; 107962 protein sequences
- **Environment**: Dawn 6000A
  - **One Core**
    - **Time**: estimate 6 years
  - **677 Fermi C2050**
    - **Time**: 2.034 h
Seismic Wave

- SORD is an open-source software developed by Geoffrey Ely from USC, to simulate 3D wave propagation and spontaneous rupture on hexahedral mesh.
- Supports many types of BC including PML.
- The test we implemented involved two layers, one (7km) over another (1km) with rectangular mesh. A double-coupled point is set at (0, 0, 2km) and last for 0.1 second to provide seismic waves. Seismic wave propagates in the whole space during the test. Two types of waves will be observed, P wave and S wave.
- Based on Emmett and David Wang’s work which outlined a framework. Tim Dong do some optimization and MPI+CUDA implementation.

1000 steps on NVIDIATesla 1060C and Xeon X5570 2.9GHz
C4: Computational Cosmology Consortium of China
Who we provide our service to

- CAD/CAE engineers

What we deliver to them

- A high-performance service
  - DeepComp 7000 for parallel solver
  - High-performance graphic workstations for pre/post processing
- A high-usability cloud computing solution via internet
  - Remote graphical access to workstations
  - Grid-computing based resources
  - Web portal integrated with CAE software
- A high-safety environment
  - Secure access through VPN and firewall
  - Isolate unauthorized access from cluster by web portal
Fingerprint Recognition

- **Fingerprint database**: 19,600,000 fingerprints
- **HPC**: 1024 cores (16 nodes, 64 cores/node)
- **Speed**: 4000 fingerprints/second/core
- **Run time**: 3 months (linear Speedup)
**SCE Introduction**

- **SCE** is an acronym for
  - Scientific, Super, Scalable
  - Computing
  - Environment, Easy, Yi

**Yì:** have 10+ meanings in Chinese

- change (改变)
- easy (容易)
- the Book of Changes (周易)
- ...

Some pictures in this slide are from the Internet.
SCE Introduction

- **Change we need**
  - **Simple**
    - ✓ many HPCs as one
  - **Easy**
    - ✓ bring input, take result
  - **Stable**
    - ✓ jobs can run anytime
GridMol

A Molecular Visualizer and Builder by SCCAS
Overview

- Developed by Virtual Laboratory for Computational Chemistry, SCCAS
- A typical application of SaaS (Software as a Service) for molecular modeling and visualization
- An extensible tool for building a high performance computational chemistry platform in Grid environment
- Providing users one-stop calculation service
Functions

- Molecular Modeling
- Molecular Visualization
- Calculation results analysis
- Job submission and monitoring
Workflow of CryoEM technique

CryoEM

Biologist

2d images

reconstruction

3d density map

Analysis of 3d density map (visualization, segmentation, fitting)
Motivation

Visualization

Segmentation

Structure fitting
Features

- Volume rendering for density maps
- Automatic Segmentation
- Automatic fitting for multi-crystal structures
- Easy movie made based on key frame
China Scientific Computing Grid (China ScGrid)
## GPU Clusters within CAS

<table>
<thead>
<tr>
<th>Site</th>
<th>Vendor</th>
<th>$R_{\text{peak}}$ /Tflops</th>
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</thead>
<tbody>
<tr>
<td>Institute. of Electrical Engineering</td>
<td>Lenovo</td>
<td>112</td>
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<tr>
<td>Shenzhen Institutes of Advanced Technology</td>
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<td>200</td>
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<td>USTC</td>
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<td>CNIC</td>
<td>Lenovo, Dawning</td>
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<td>Institute of Geology and Geophysics</td>
<td>Lenovo, Dawning</td>
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<tr>
<td>Institute of Modern Physics</td>
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<tr>
<td>SUM</td>
<td></td>
<td>1.914 Pflops</td>
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</tbody>
</table>
Acknowledgements

- My colleagues
  - Long Wang, Haili Xiao, Zhong Jin, Guihua Shan, Zhonghua Lu, etc.

- My Students
  - ...
Question & Suggestion

Thank you very much!