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

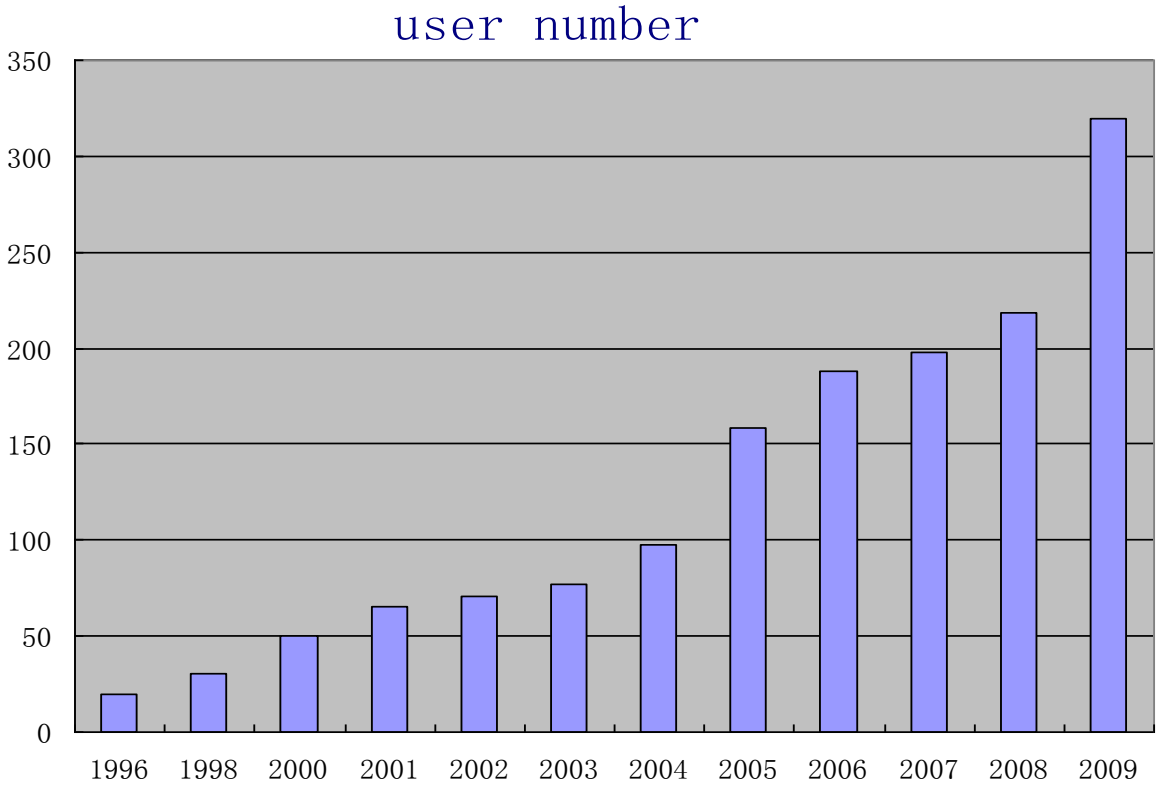
- **During 1996-2000 (9th 5 year plan)**
  - In 1996, SGI Power Challenge XL
    - ✓ 6.4Gflops
    - ✓ 16 CPUs
  - In 1998: Hitachi SRR201
    - ✓ 9.6GFlops
    - ✓ 32CPUs
  - **In 2000, Dawning 2000 II**
    - ✓ 111.7Gflops
    - ✓ 164 CPUs

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)



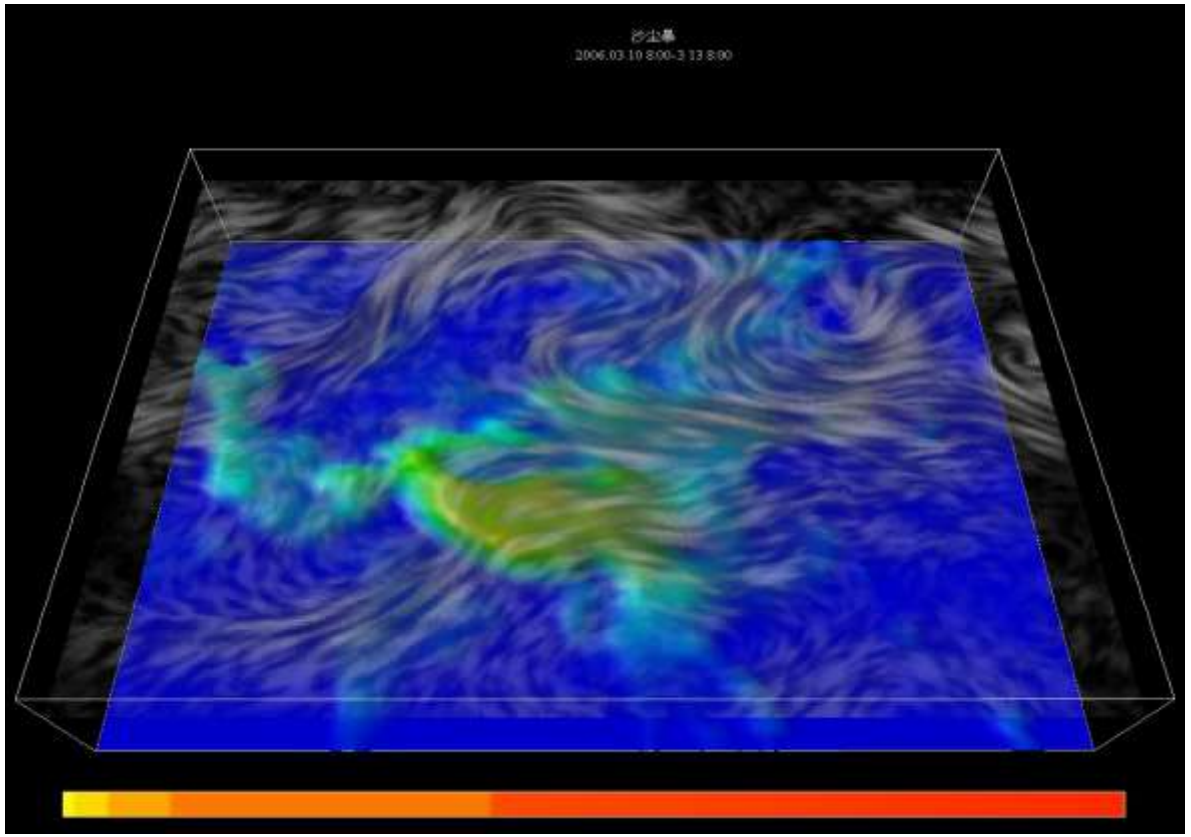
SCCAS-R&D of Algorithms and software

- 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

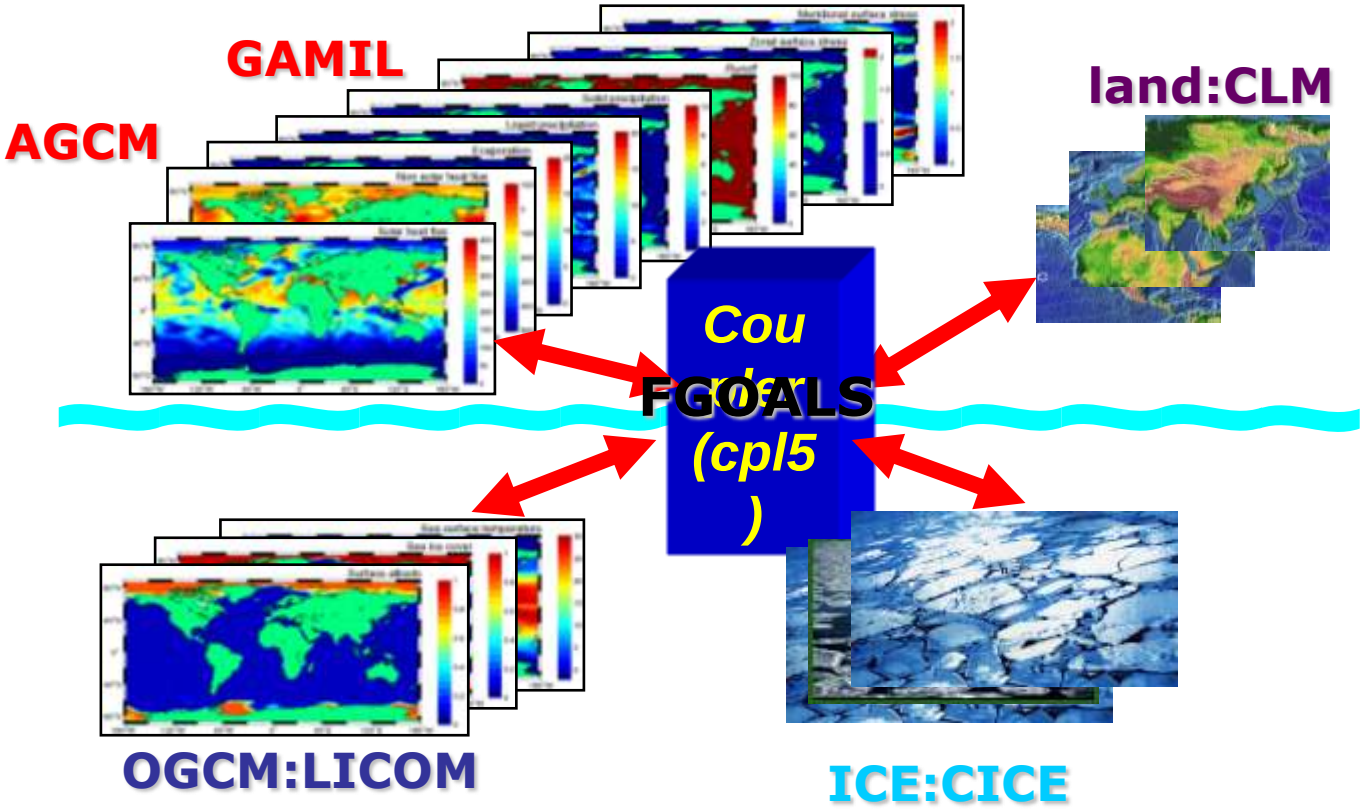
Prediction of Sandstorm

- **Real-time prediction system of Sandstorms in China Meteorological Bureau**
- **DeepComp6800**
  - 256 CPUs
  - from 15hours

  down to 8mins



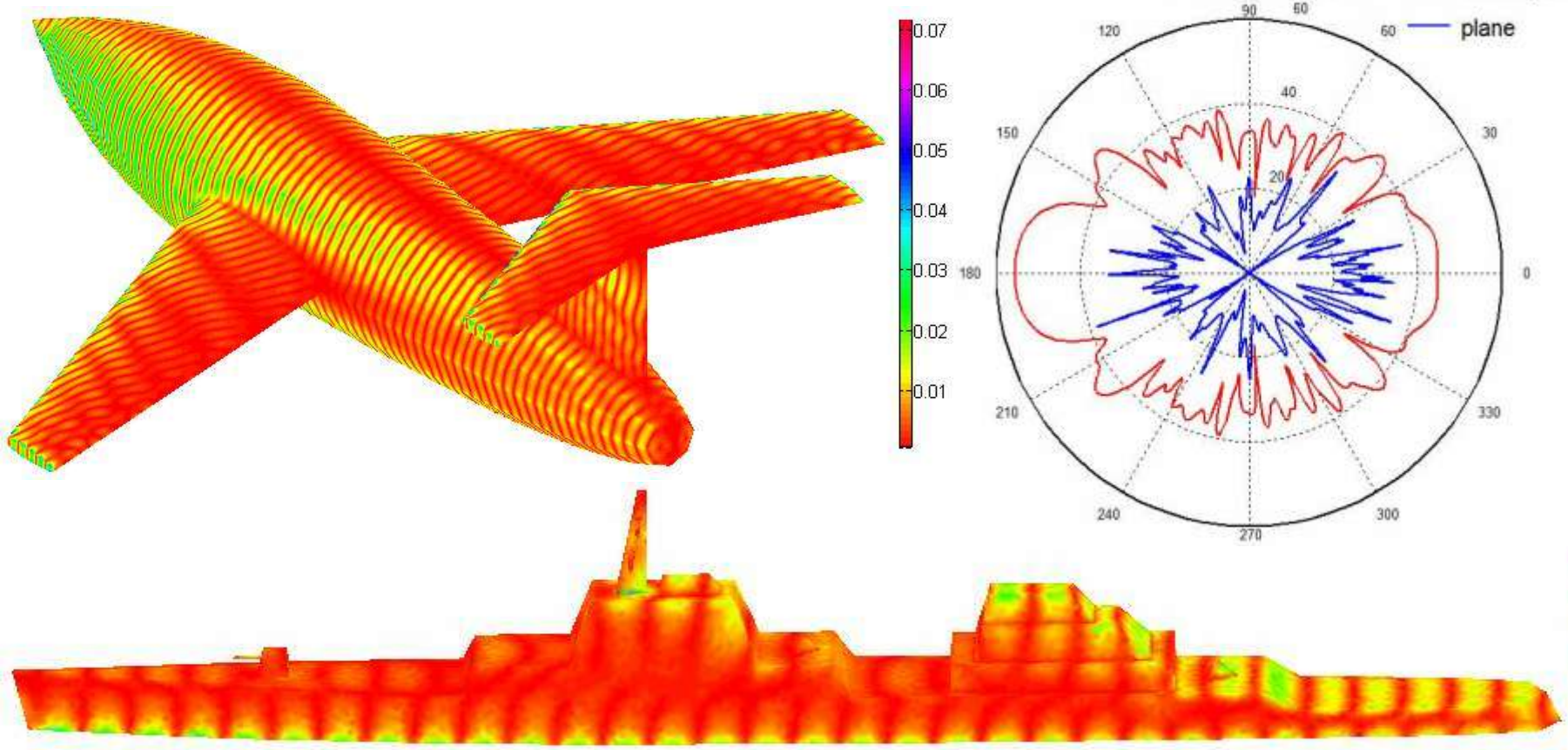
Global Climate Model-FGOALS



CPU	AGCM	LAND	OGCM	ICE	Coupler
1620	720	90	540	180	90

EM Scattering

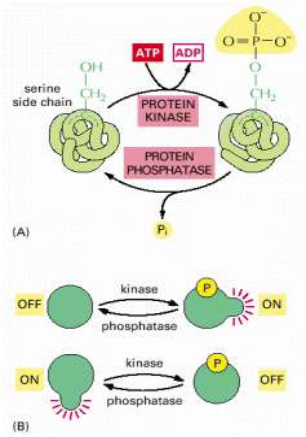
- **The surface currents and RCS of plane and destroyer models**
  - Used for antenna design, RCS analysis
  - Stealth design of airplanes, etc.

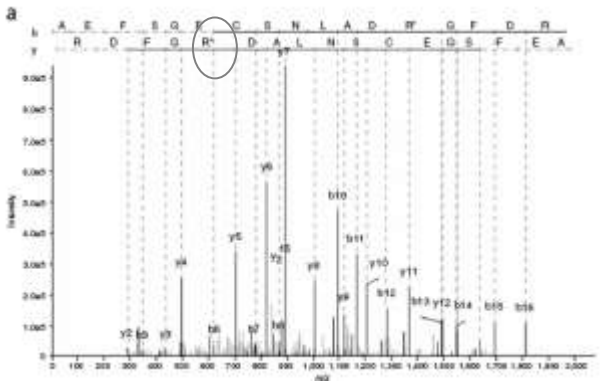


P_InsPecT/cuda-InsPecT Software

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

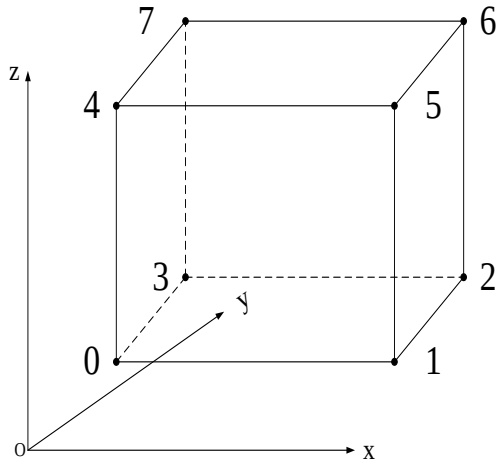
	One Core（estimate）	2048 Cores
Time	1177.7 h	0.4 h

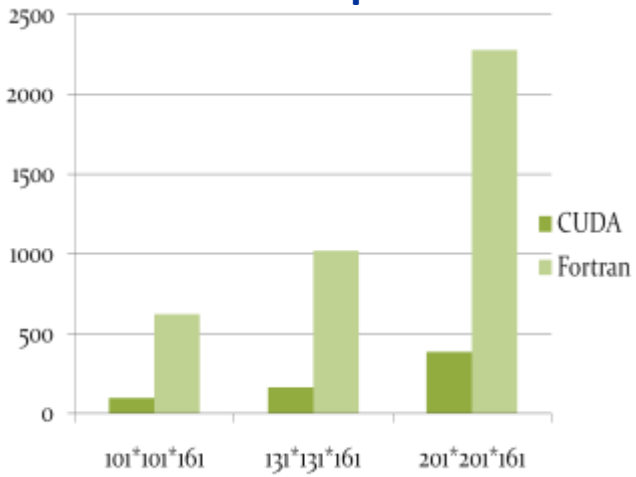
Software：cuda-InsPecT（two modifications）
Database：62346 mass spectrometric;
107962 protein sequencesE
Environment：Dawn 6000A

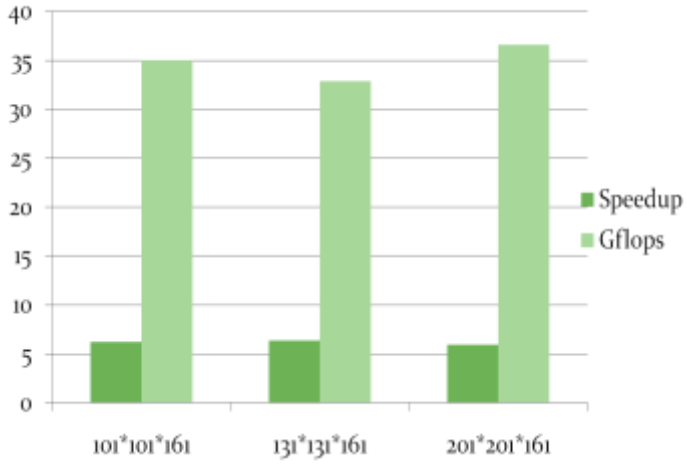
	One Core（estimate）	677 Fermi C2050
Time	6 years	2.034 h

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.



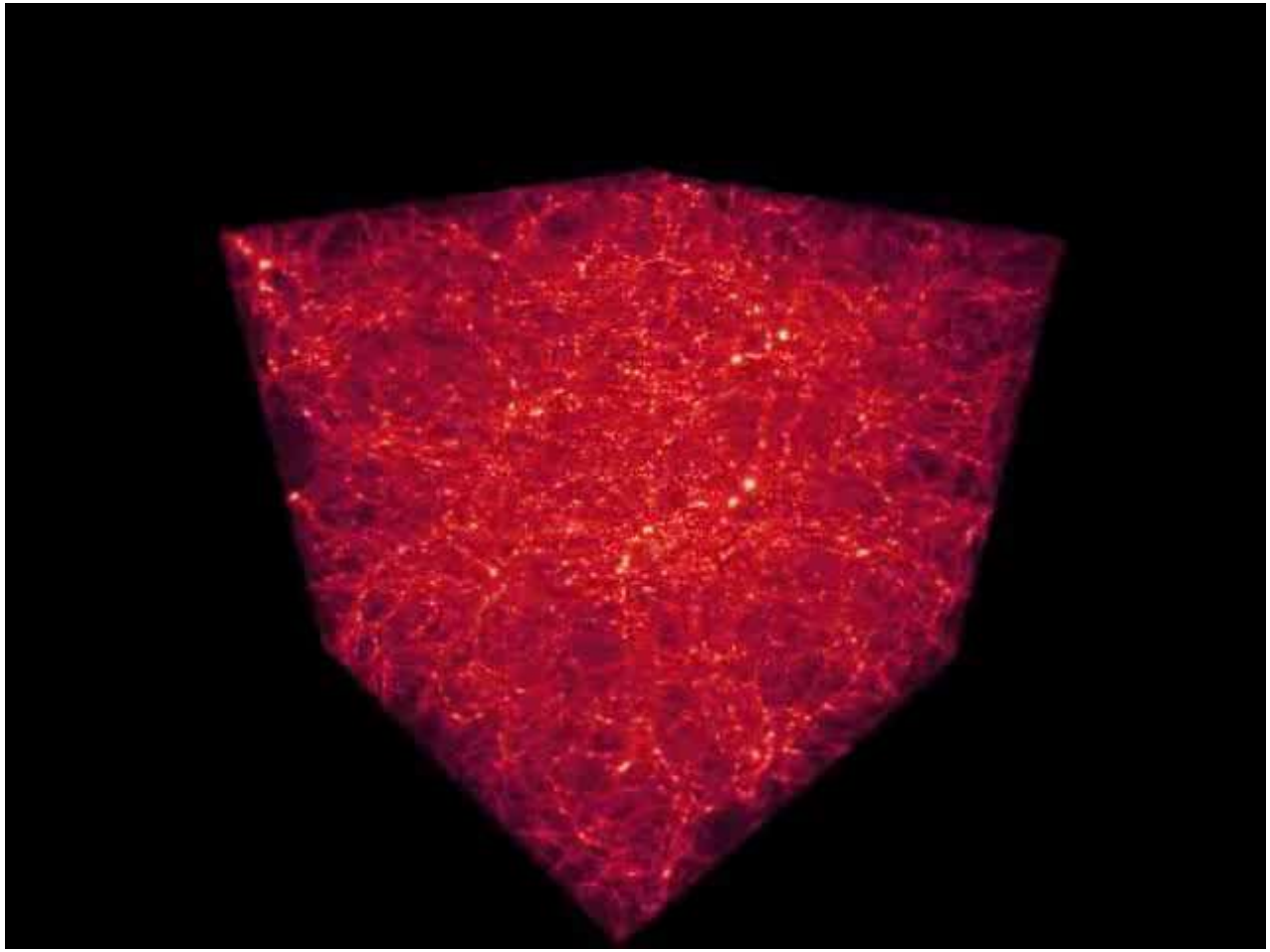




cubic stencil

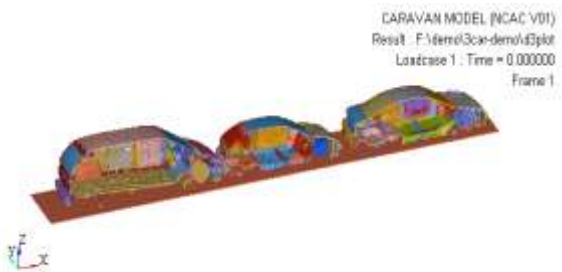
1000 steps on NIVIDIA Tesla 1060C and Xeon X5570 2.9GHz

C4: Computational Cosmology Consortium of China

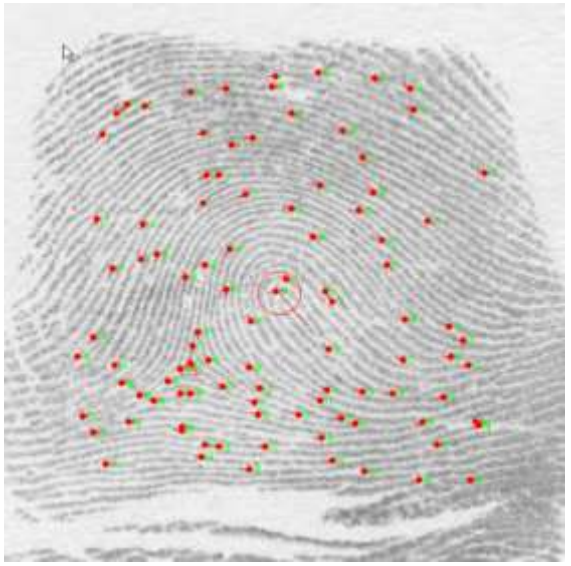


CAD/CAE Platform in Automation Industry

- **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 por



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, Yì

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

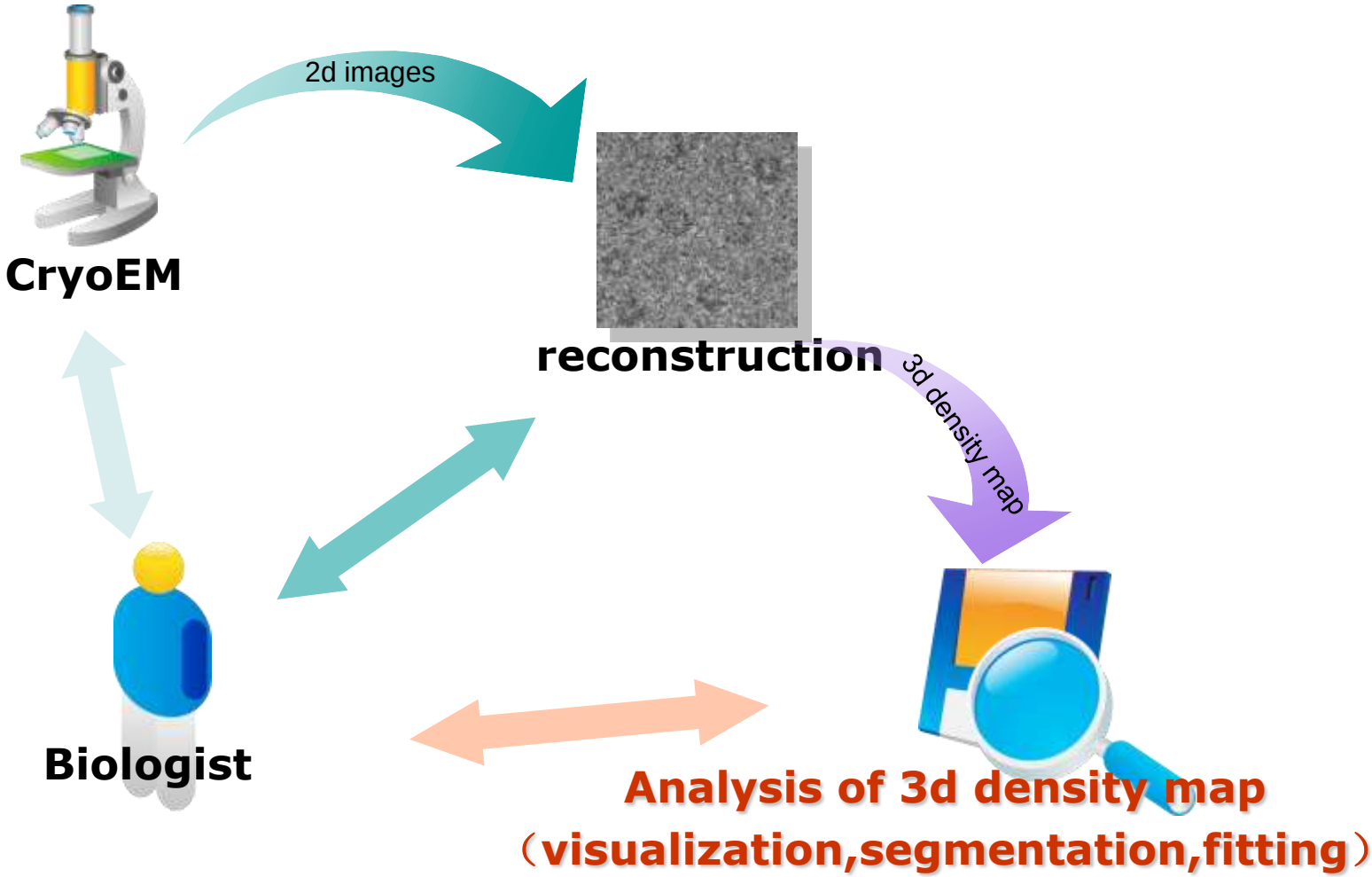
Overview

- **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**

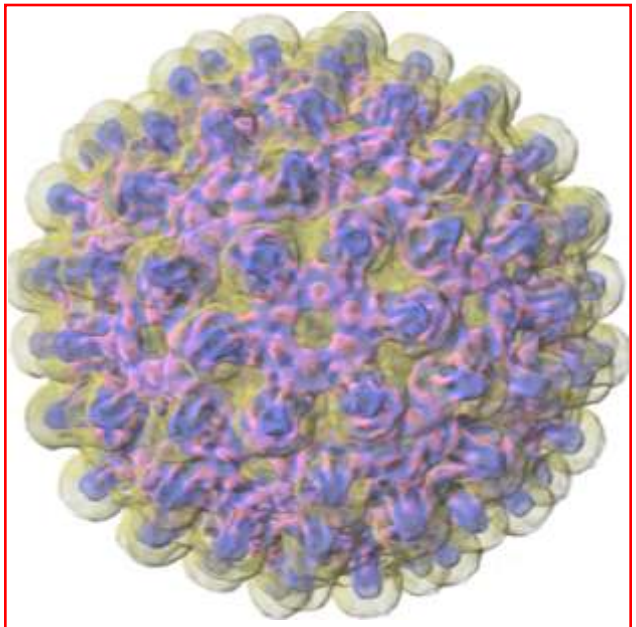
Functions

- **Molecular Modeling**
- **Molecular Visualization**
- **Calculation results analysis**
- **Job submission and monitoring**

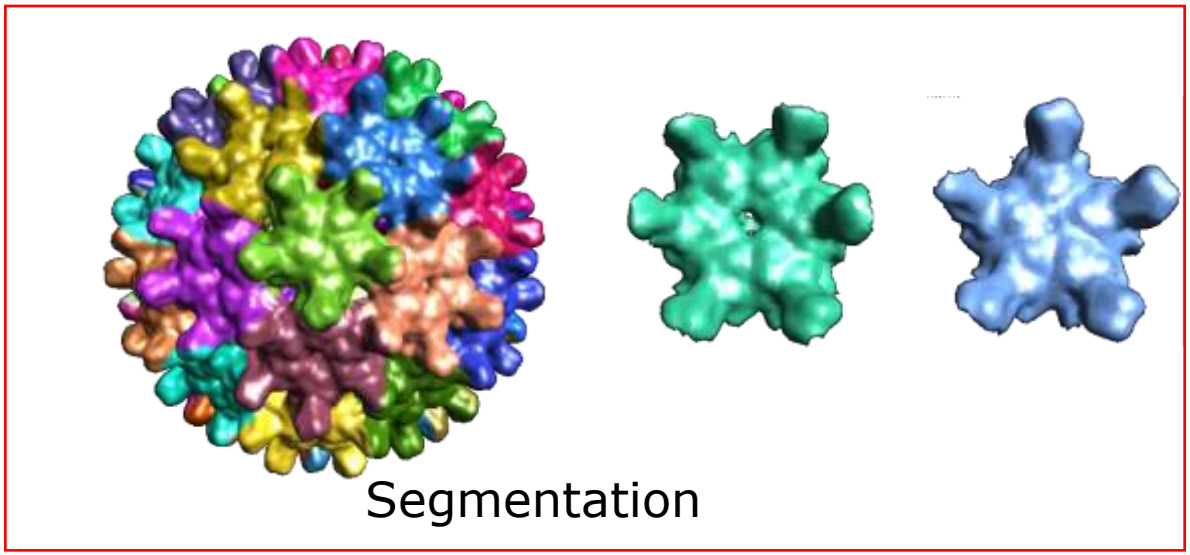
Workflow of CryoEM technique



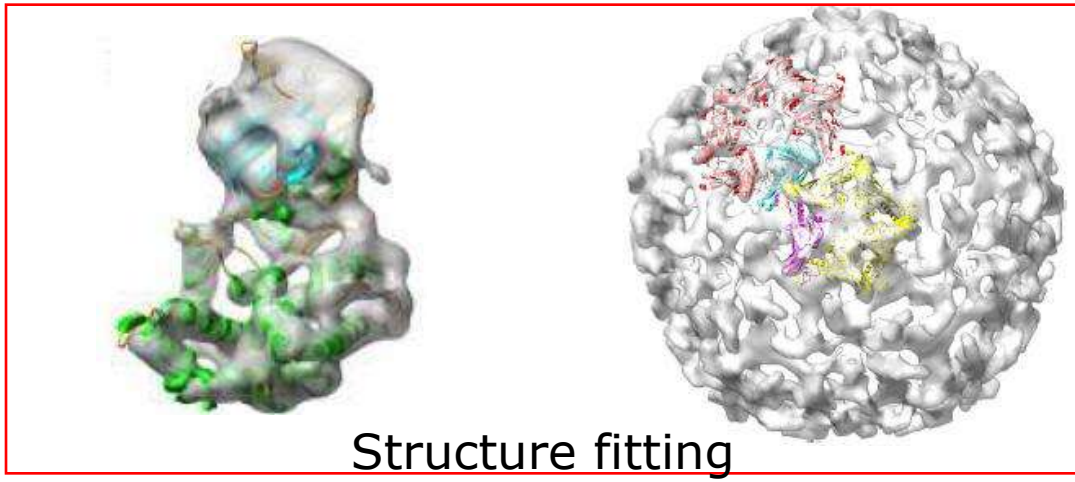
Motivation



Visualization



Segmentation

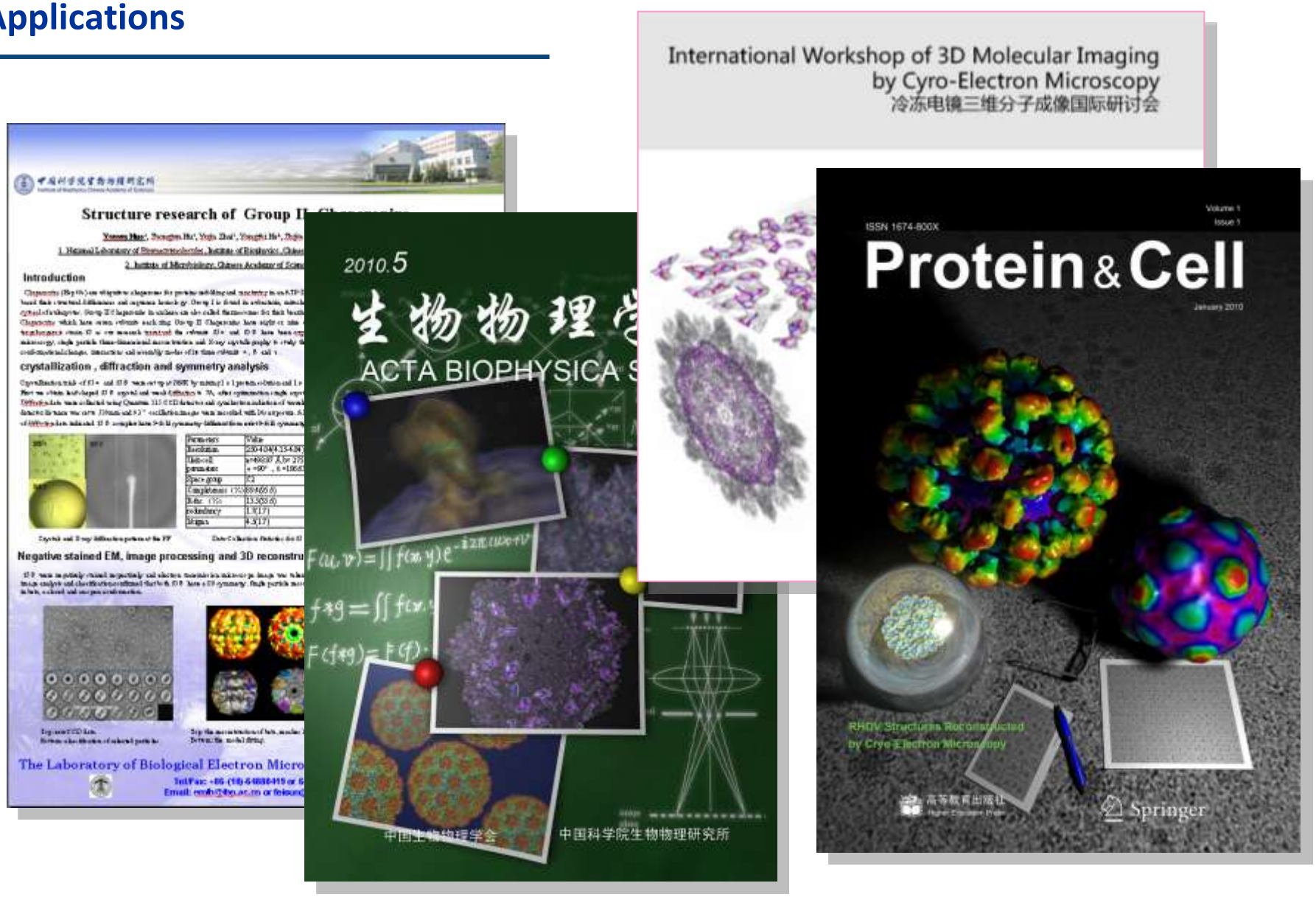


Structure fitting

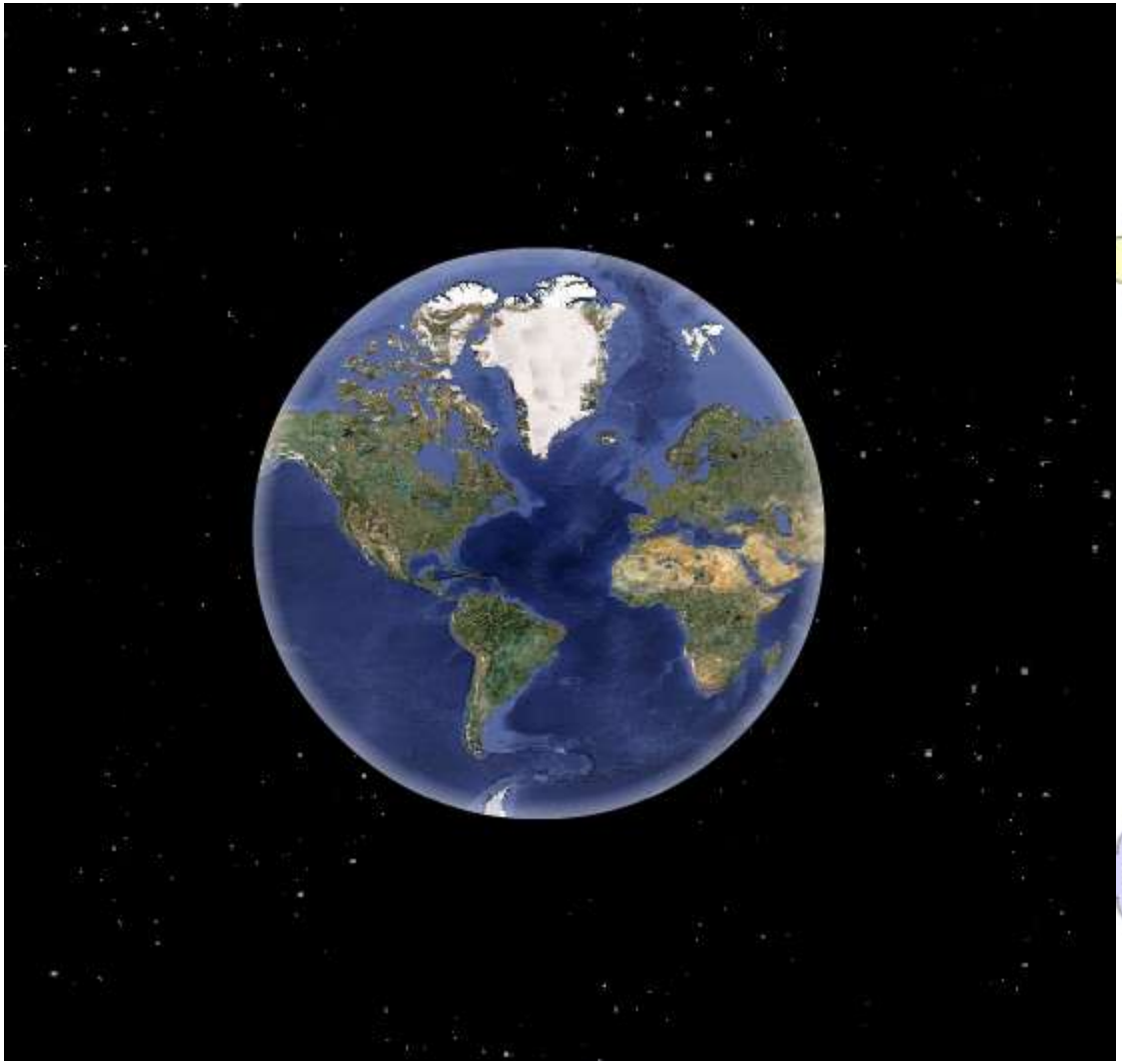
Features

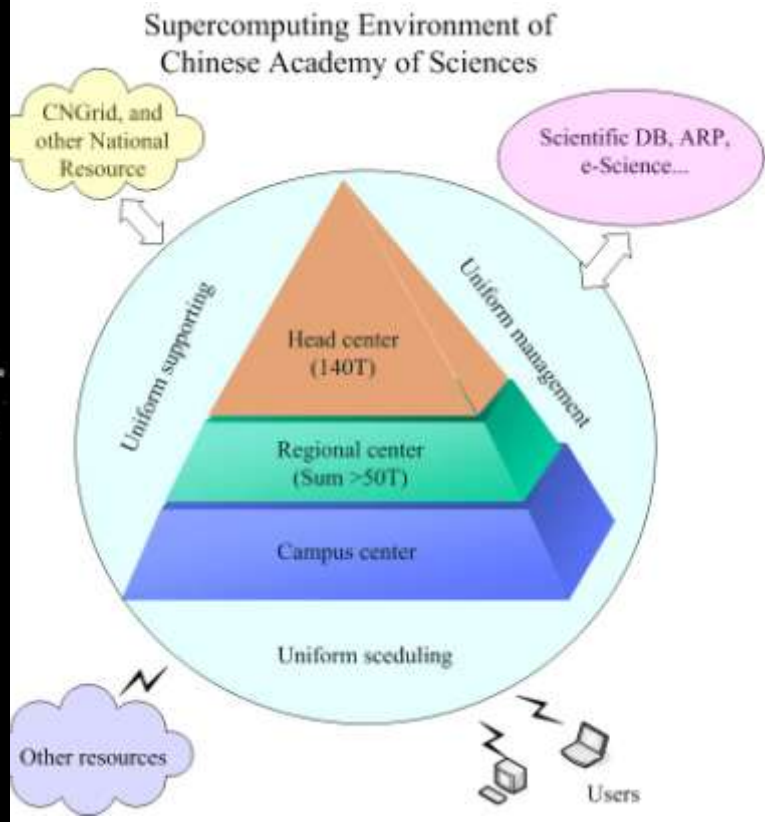
- Volume rendering for density maps
- Automatic Segmentation
- Automatic fitting for multi-crystal structures
- Easy movie made based on key frame

Applications



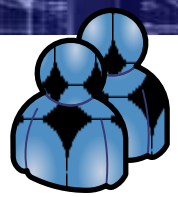
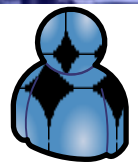
China Scientific Computing Grid (China ScGrid)





GPU Clusters within CAS

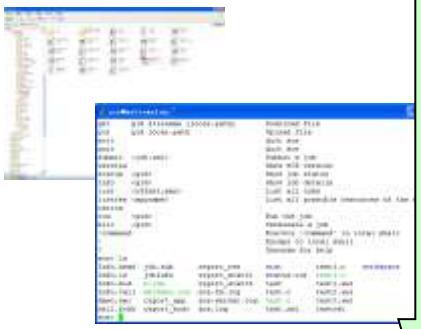
Site	Vendor	R_{peak} /Tflops
Institute. of Electrical Engnineering	Lenovo	112
Shenzhen Institutes of Advanced Technology	Lenovo	200
USTC	Lenovo	183
CNIC	Lenovo, Dawning	300
National Astronomical Observatories	Lenovo	158
Institute of Geology and Geophysics	Lenovo, Dawning	200
Institute of Modern Physics	Lenovo	202.5
Institute of High Energy Physics	Dawning	195.5
Institute of Metals Research	Dawning	183
Purple Mountain Observatory	Dawning	180
SUM		1.914 Pflops

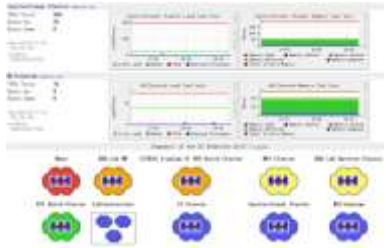



Users Administrator

Windows / Linux Clients

Web Portal



SCE Middleware



HPC, Cluster, Workstation, Storage

Acknowledgements

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

Question & Suggestion

Thank you very much!