The Path to Petascale Computing in China

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Outline

□ **Overview the HPC History of China**

□ **Brief Introduction of SCCAS**

□ **Grid environment overview**

□ **Applications in science and engineering**

□ **Future Plan on high performance environment**

Overview the HPC History of China

1. Started in the late of 1980's

2. Developing in the 1990's

Parallel computers (1988-1994)

□ **BJ-01 (1988-1992)**

– 4 processors, with global and local memmory, made by ICT, CAS

□ **Transputers (1991-1994)**

– Several parallel systems, our group had a 17 transputer system

□ **KJ 8950 (1993-1995)**

– 16 processors, with global and local memmory, made by ICT, CAS

□ **1995 1st parallel computer Dawning 1000 occurred**

– Peak performance 2.5GFLOPS in single precision, HPL 50%

– Similar to Paragon machine, NX parallel implementation environment

– Intel i860

National High Performance computing Centers (1996-2000)

- **National High Performance computing Center (Beijing)**
  - In Institute of computing technology, CAS
- **National High Performance computing Center (Wuhan)**
  - Huazhong University of Science and Technology
- **National High Performance computing Center (Chengdu)**
  - Southwest Jiaotong University
- **National High Performance computing Center (Hefei)**
  - University of Science and Technology of China

- **Supercomputing Center in Chinese Academy of Sciences (SCCAS)**
  - 1996
- **Shanghai Supercomputing Center (SSC)**
  - 2001

Clusters (2001-2005)

❑ **Lenovo DeepComp 6800 (SCCAS)**

- 2003, top500 rank 14th, peak performance 5.2TFLOPS

- Itanium II, Linux OS, MPI, QsNet

- Budget 60M RMB

  ✓ MOST 15M, Lenovo 15M, CAS 30M

❑ **Dawning 4000 (SSC)**

- 2004, top500 rank 10th, peak performance 11 TFLOPS

- AMD Opteron, Linux Os, MPI, Merinet 2000

- Budget 60M RMB

  ✓ MOST 30M, Shanghai Government 30M

❑ **Many other clusters installed during that period**

100TFLOPS HPCs (2006-2010)

- **Lenovo DeepComp 7000**
  - 150TFLOPS, our center, Dec., 2008
  - Budget 180M RMB
    - ✓ MOST 80M, Lenovo 25M, CAS 75M

- **Dawning 5000**
  - Peak performance 200TFLOPS, AMD processors
  - Aug., 2009, in Shanghai Supercomputing Center
  - Top500 rank 10th on June of 2009
  - Budget 200M RMB
    - ✓ MOST 100M, Shanghai Government 100M
  - Software and environment
    - ✓ 100M

Peta Flops HPCs

☐ **Dawning Nebulae**
- 600TFLOPS CPU + 3PFLOPS GPU
- Top500 Rank 2nd
- Budget 600M RMB
  - ✓ MOST 200M, Shenzhen Government 400M
- Upgrade 1PFLOPS CPU, 200 TFLOPS Godson

☐ **NUDT Tianhe**
- 200TFLOPS CPU + 1.2PFLOPS GPU
- Top500 rank 7th
- Budget 600M RMB
  - ✓ MOST 200M, Tianjin Government 400M
- Upgrade 1PFLOPS CPU + 4PFLOPS GPU
  - ✓ HPL 2.5PFLOPS

Brief Introduction of SCCAS

1. Providing computing power and technical support for scientists

2. Training in HPC algorithm and programming

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)

user number
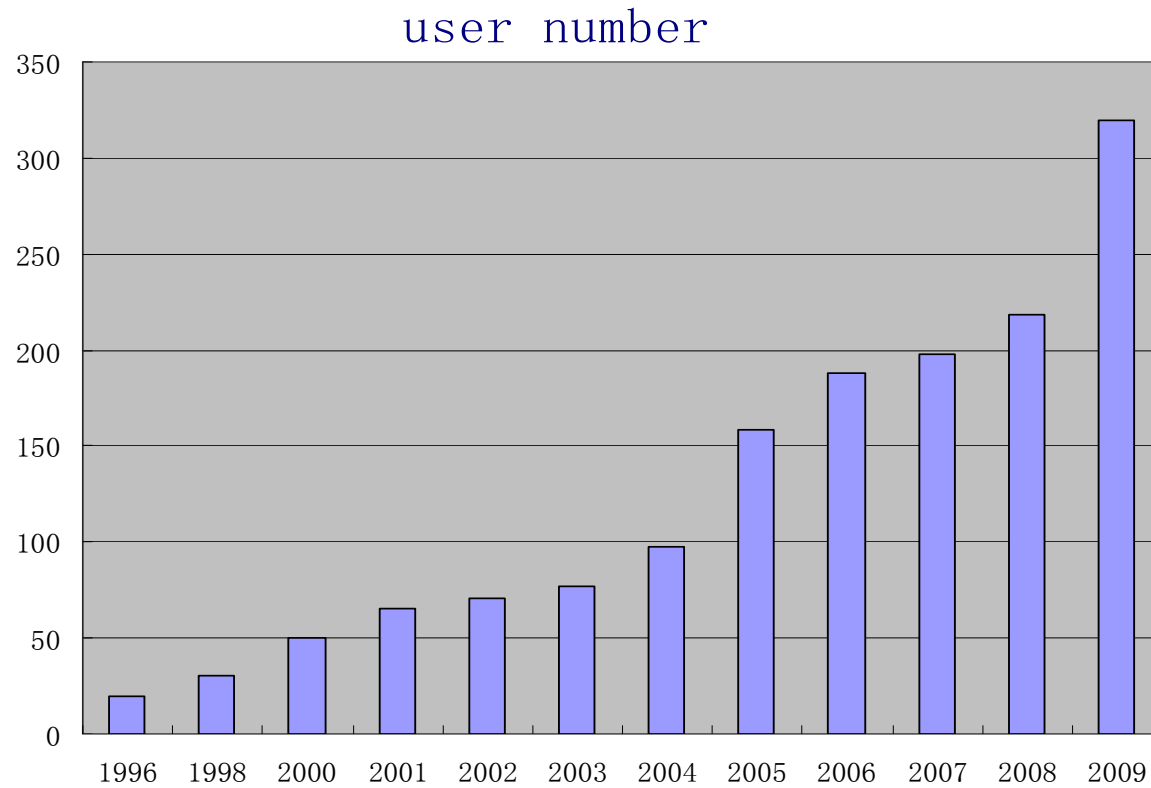
SCCAS-R&D of Algorithms and software

- **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**

# Grid environment overview

1. China National Grid (CNGrid)
2. China Scientific Computing Grid (ScGrid)

China National Grid

China National Grid

- **CNGrid operation center**
  - Supercomputing center of CNIC of CAS
- **Northern major node**
  - Supercomputing center of CNIC of CAS
- **Southern major node**
  - Shanghai supercomputing center
- **Normal nodes**
  - 9 sites, they are Tsinghua University, Beijing Institute of Applied Physics and Computational Mathematics, Shandong University, University of Science and Technology of China, Huazhong University of Science and Technology, Shenzhen Institute of Advanced Technology of CAS, Hong Kong University, Xi'an Jiaotong University, Gansu province Supercomputing Center

China Scientific Computing Grid (ScGrid)

Supercomputing Environment of Chinese Academy of Sciences

CNGrid, and other National Resource

Scientific DB, ARP, e-Science...

Uniform supporting

Uniform management

Head center (140T)

Regional center (Sum >50T)

Campus center

Uniform sceduling

Other resources

Users
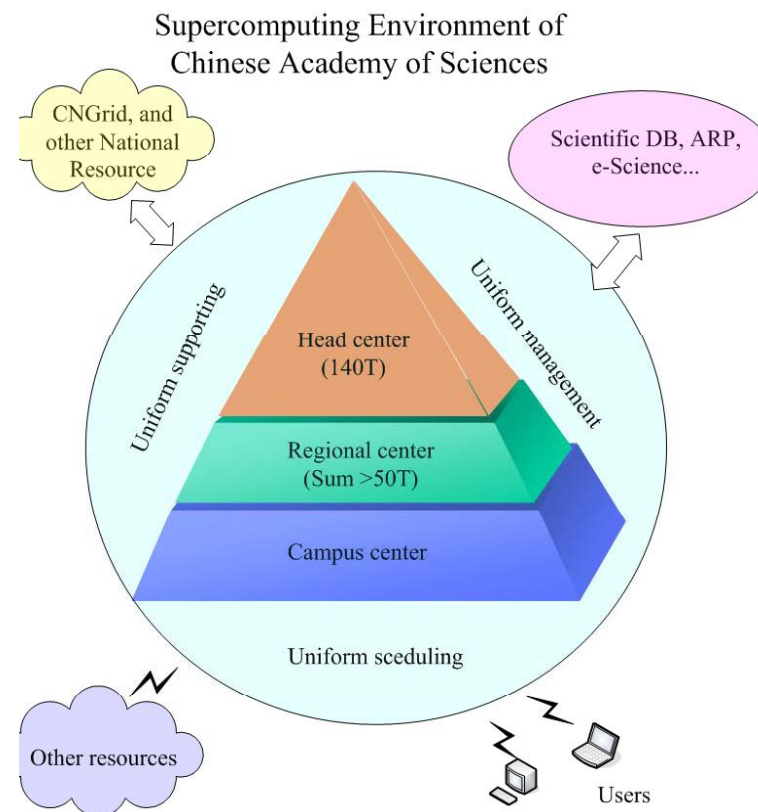
GPU Clusters within CAS

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
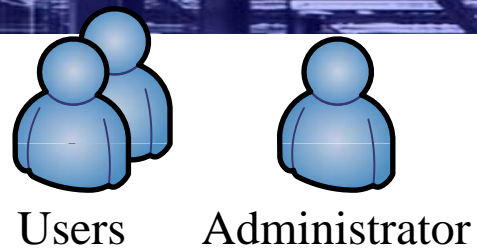
Windows / Linux Clients

Web Portal
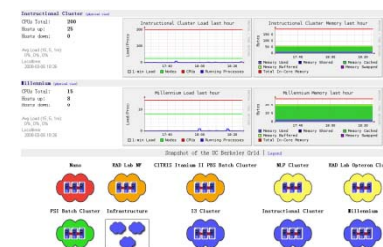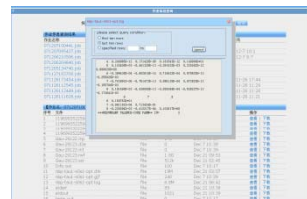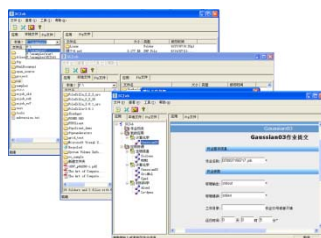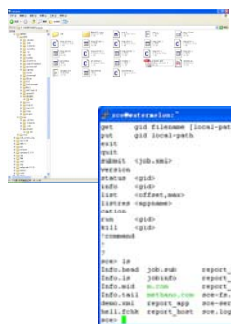
SCE Middleware
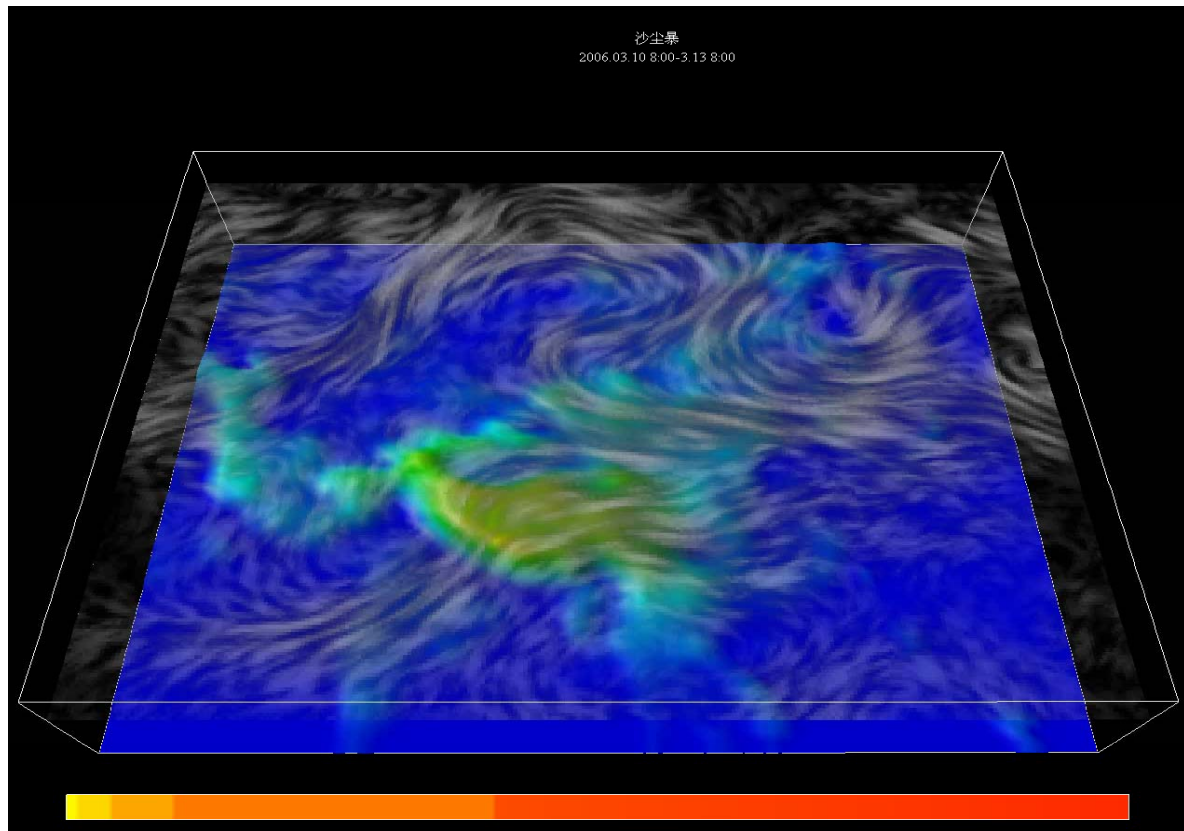
HPC, Cluster, Workstation, Storage

Applications in Science and Engineering

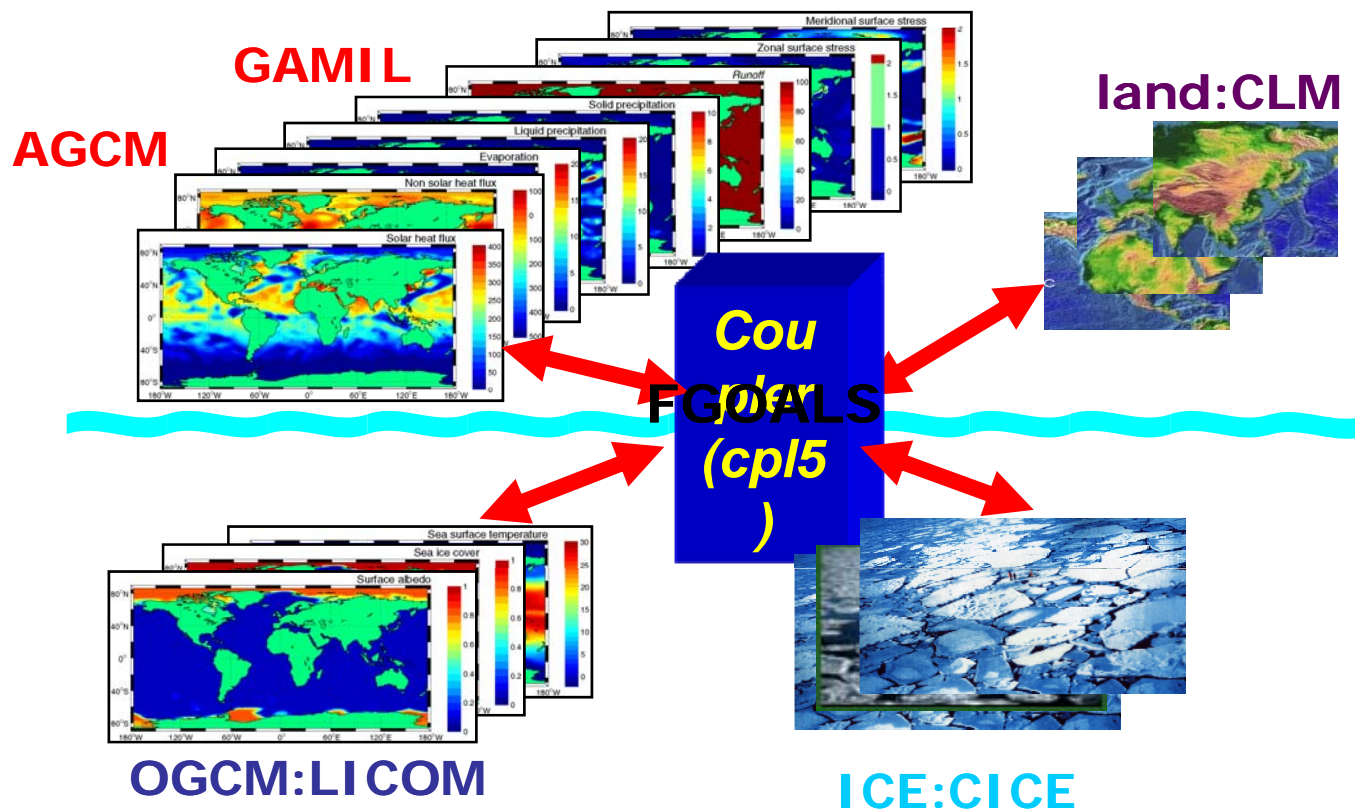1. Scientific Research

2. Industrial Computing

Prediction of Sandstorm

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

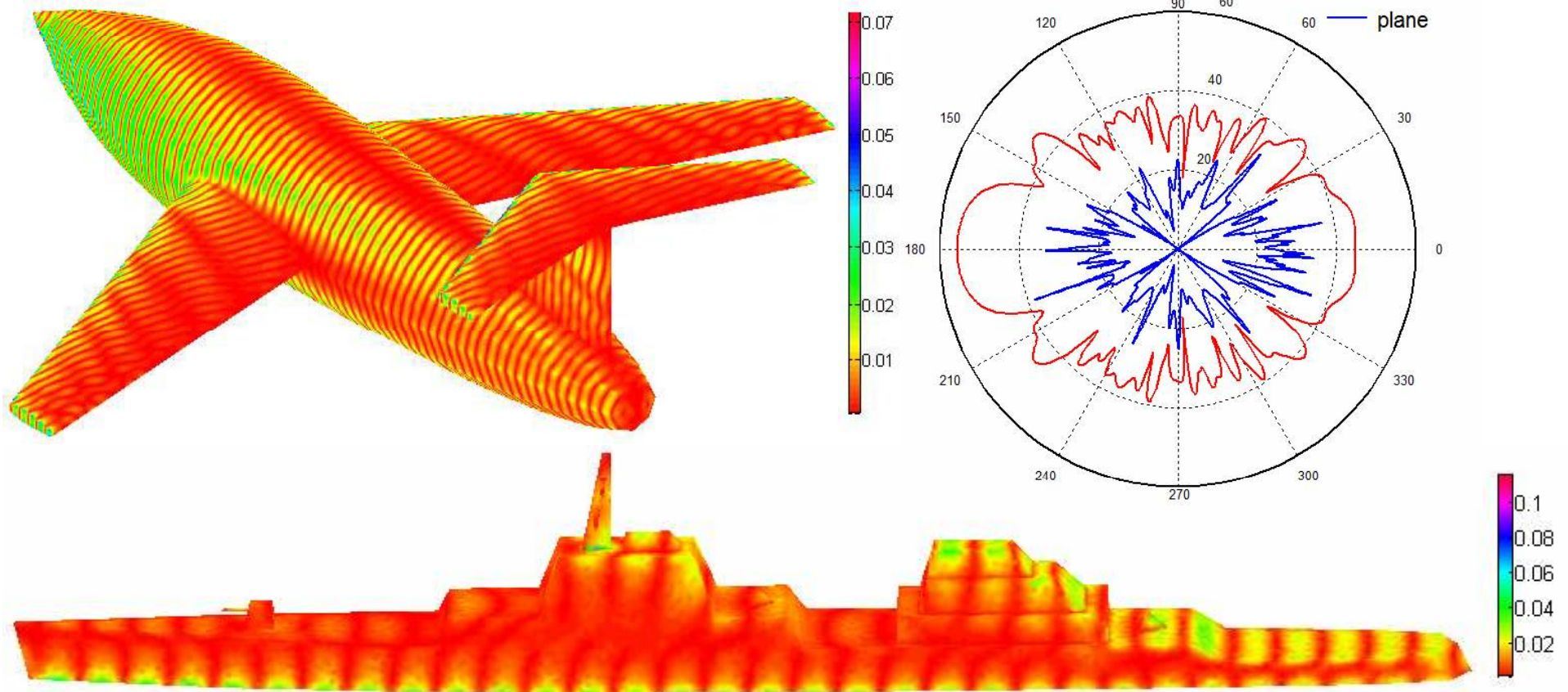   down to 8mins

Global Climate Model-FGOALS

GAMIL

AGCM

land:CLM

Coupler FGOALS (cpl5)

OGCM:LICOM

ICE:CICE

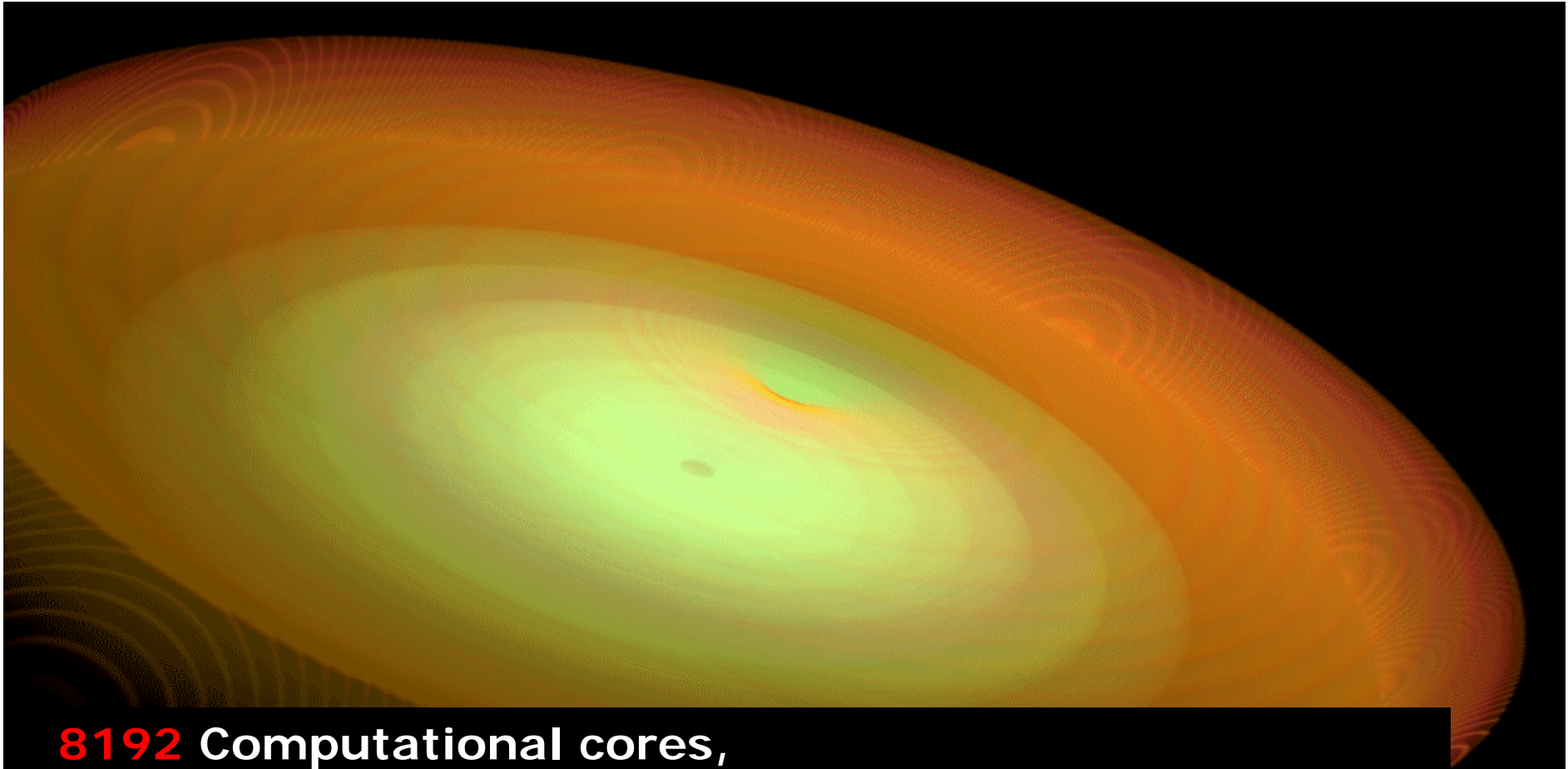| CPU	AGCM	LAND	OGCM	ICE	Coupler
1620	720	90	540	180	90

EM Scattering

□ **The surface currents and RCS of plane and destroyer models**

– Used for antenna design, RCS analysis

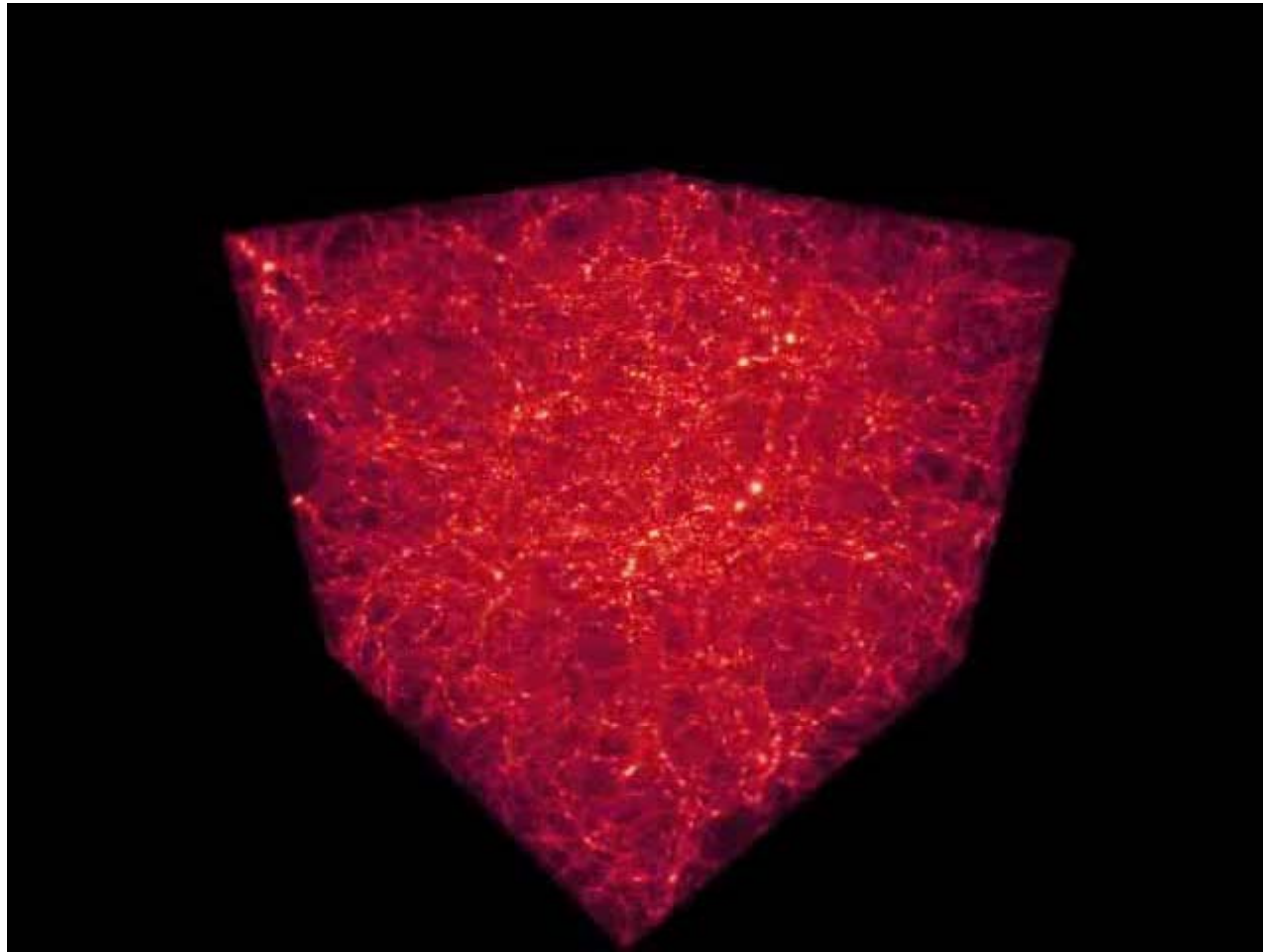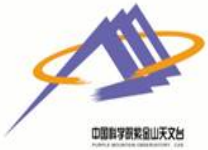– Stealth design of airplanes, etc.

Galactic Wind Simulation

8192 Computational cores,

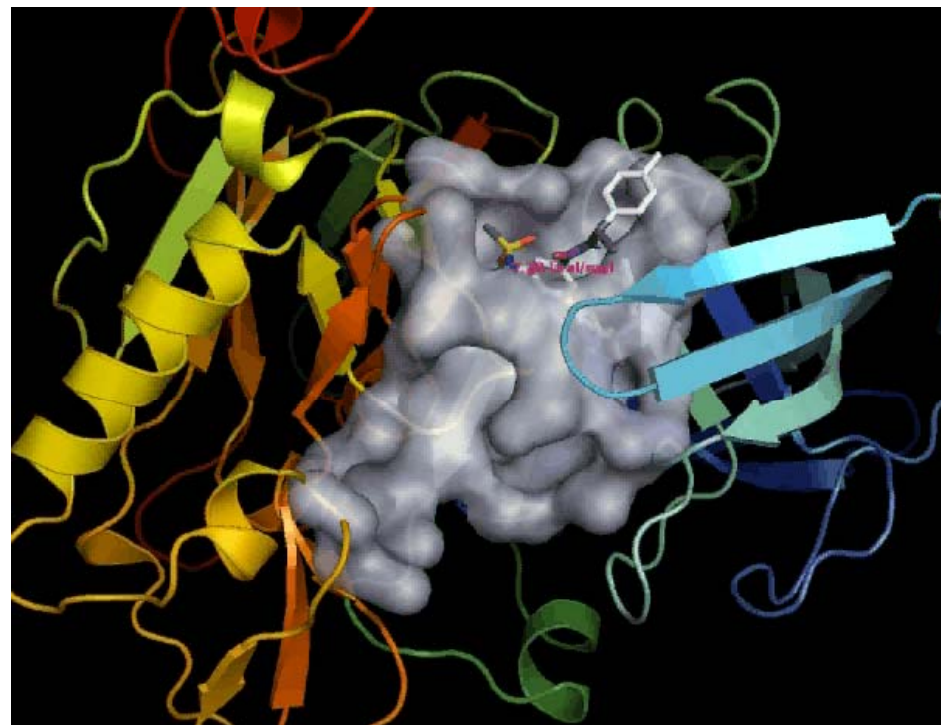Internationally advanced both in computational scale and speed
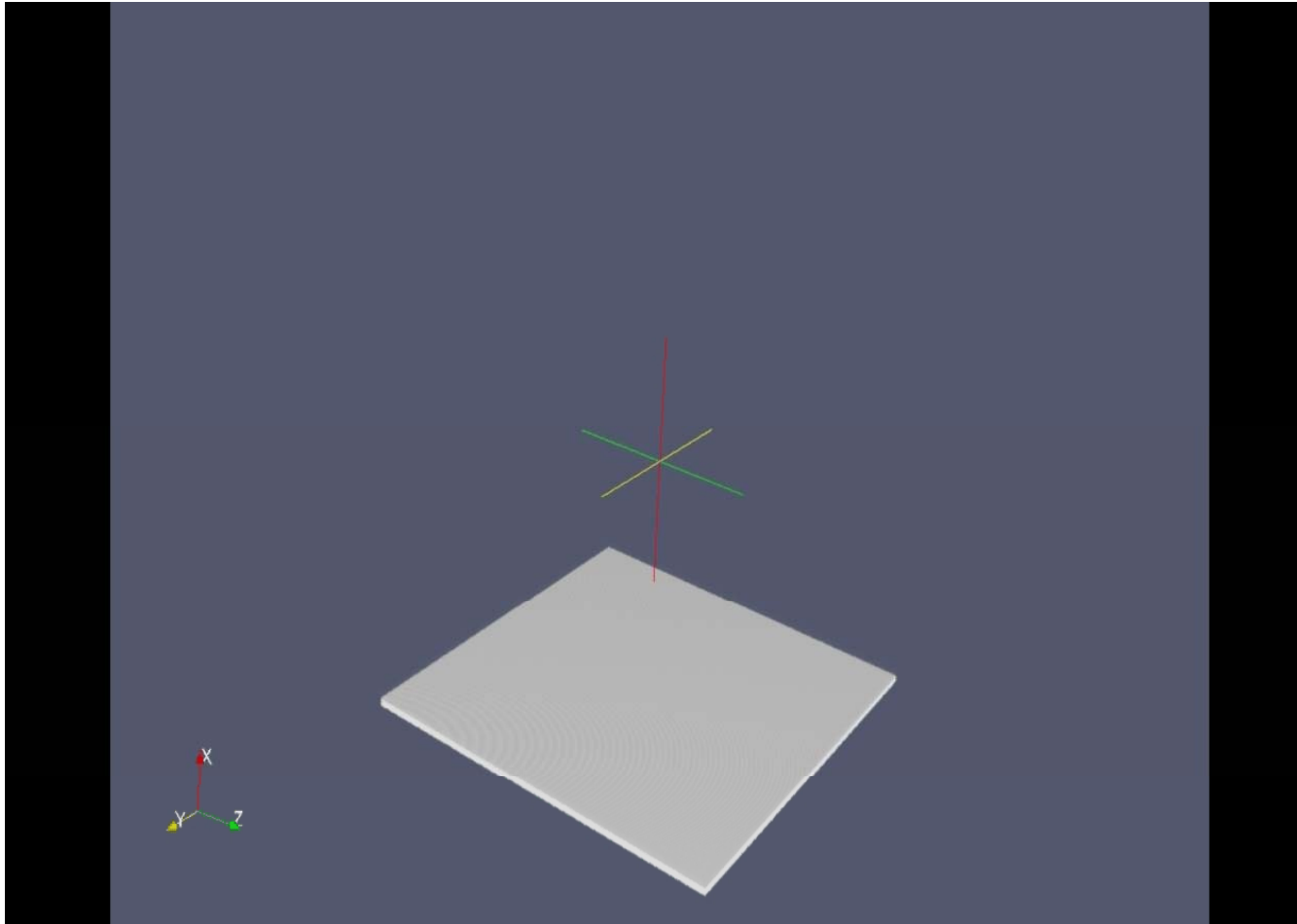
C4: Computational Cosmology Consortium of China

Drug screening for Avian Influenza

- **DeepComp7000**

- **2400 CPU cores**

- **Time consumed decreased from 2 months to 8hours**

- **The compounds screened out by this computation is forwarded to related department for further biological test**

Phase Change on Titanium Alloy

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
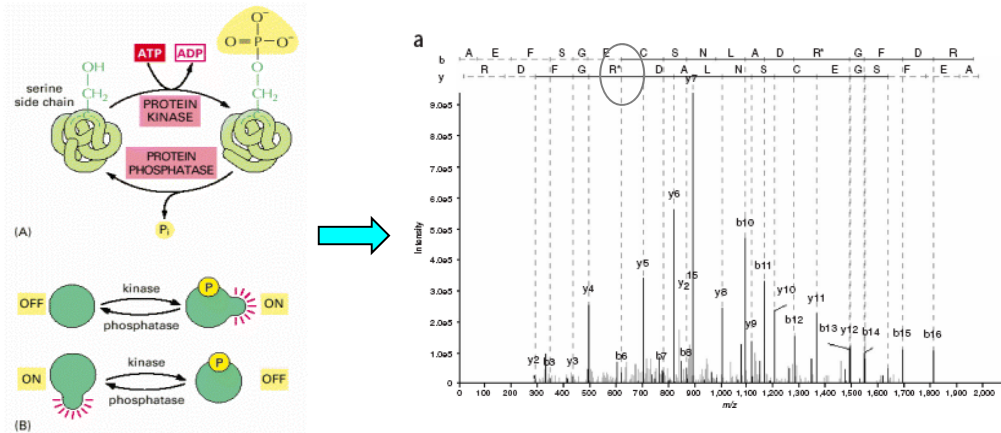
CAD/CAE Platform in Automation Industry

☐ **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 portal

CARAVAN MODEL (NCAC V01)
Result : F:\demo\3car-demo\d3plot
Loadcase 1 : Time = 0.000000
Frame 1
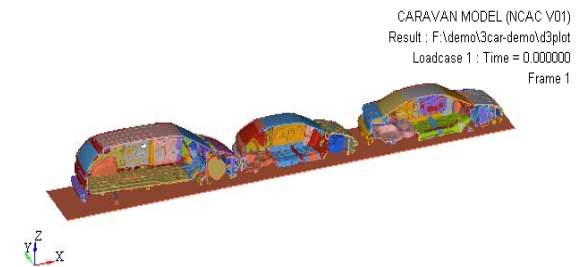
Future Plan on High Performance Environment

Petascale Supercomputers in CAS

- ☐ **1 PetaFlops computer in 2012**
  - – Budget 250M RMB
  - – For scientific computing

- ☐ **10 PetaFlops computer in 2015**
  - – Collaboration with Beijing local government
  - – Budget 700M RMB
  - – For scientific computing and industry computing

100PFlops Supercomputers in China

- **2011-2015**
  - Many peta scale HPCs
  - At least one 50-100PFLOPS HPC
  - Budget 4B RMB
    - ✓ MOST 2.4B, Local Government 1.6B
- **2016-2020**
  - 1-10ExaFLOPS HPC
  - Budget
    - ✓ Can't estimate

Question & Suggestion

Thank you very much!