
# Introduction of Supercomputing Center CNIC

**Zhong JIN**

**SuperComputing Center, CNIC, CAS**

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# Outline

- Brief Introduction to SCCAS
- Grid environment overview
- Applications in science and engineering
- Future Plan on high performance environment in CAS

# Brief Introduction to SCCAS

1. Providing computing power and technical support for scientists
2. Training in HPC algorithm and programming

# SCCAS-Computing Resources

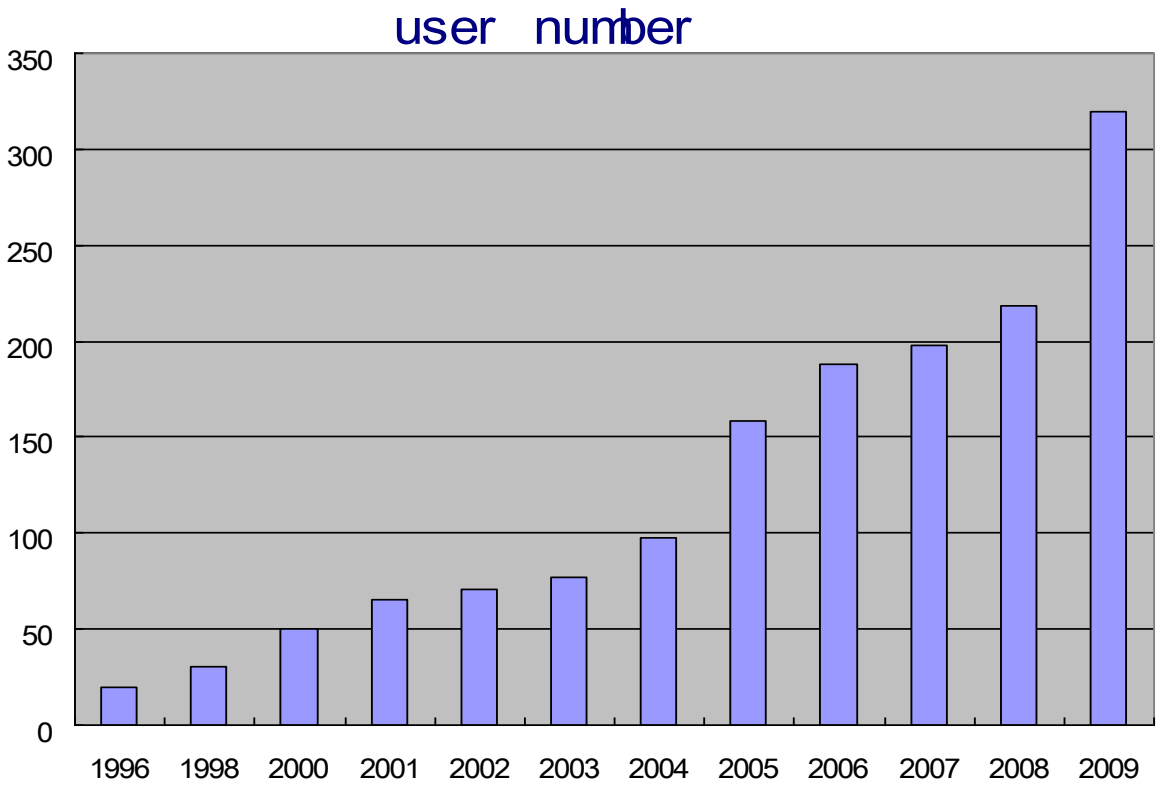
- **During 1996-2000 (9th 5 year plan)**
  - In 1996, SGI Power Challenge XL
    - ✓6.4Gflops
    - ✓16 CPUs
  - In 1998: Hitachi SRR201
    - ✓9.6GFlops
    - ✓32CPUs
  - **In 2000, Dawning 2000 II**
    - ✓ 111.7Gflops
    - ✓ 164 CPUs

# 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 2006-2010 (11th 5 year plan)**
  - In 2008, Lenovo DeepComp7000
    - ✓ 150Tflops, 13,000 cores
    - ✓ TOP500：No.19；China TOP100：No.2 (2010)
    - ✓ 3 kinds of nodes, Altix 4700, IBM 3950, IBM Blades
  - In 2009, 300TFLOPS GPU
- **During 2011-2015 (12th 5 year plan)**
  - 1 Petaflops Supercomputer is planned

# 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

# Grid environment overview

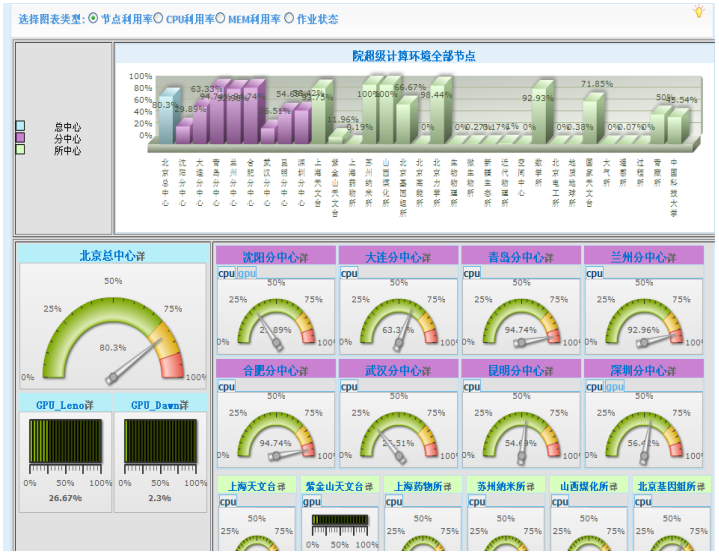
1. China National Grid (CNGrid)
2. China Scientific Computing Grid (ScGrid)

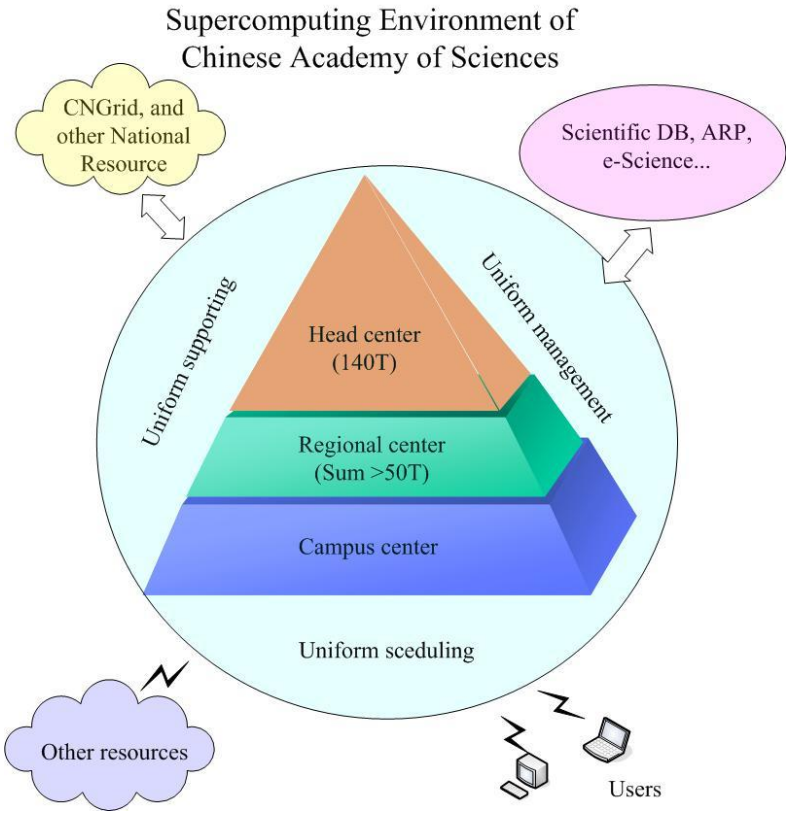
# China National Grid

# 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

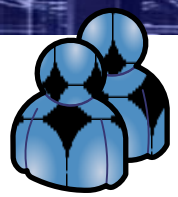
# China Scientific Computing Grid (ScGrid)

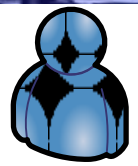



# GPU Clusters within CAS

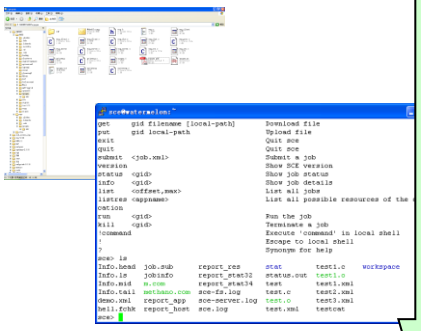
| Site | Vendor | $R_{peak}$ /Tflops |
|---|---|---|
| Institute. of Electrical Engnineering | Lenovo | 112 |
| Shenzhen Institutes of Advanced Technology | Lenovo | 200 |
| USTC | Lenovo | 183 |
| CNIC | Lenovo, Dawning | 300 |
| National Astronomical Observatories | Lenovo | 158 |
| Institute of Geology 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 |

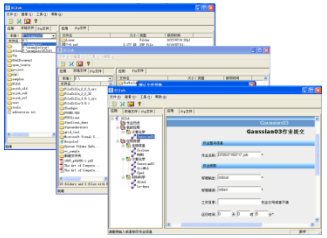

Users

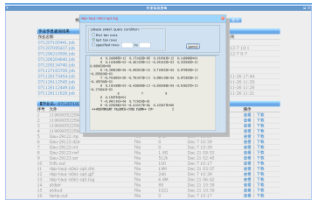

Administrator

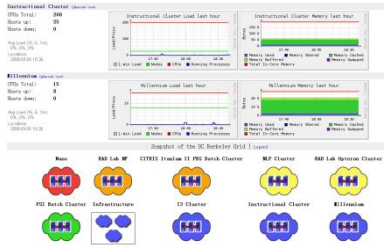
**Windows / Linux Clients**

**Web Portal**









**SCE Middleware**

HPC, Cluster, Workstation, Storage

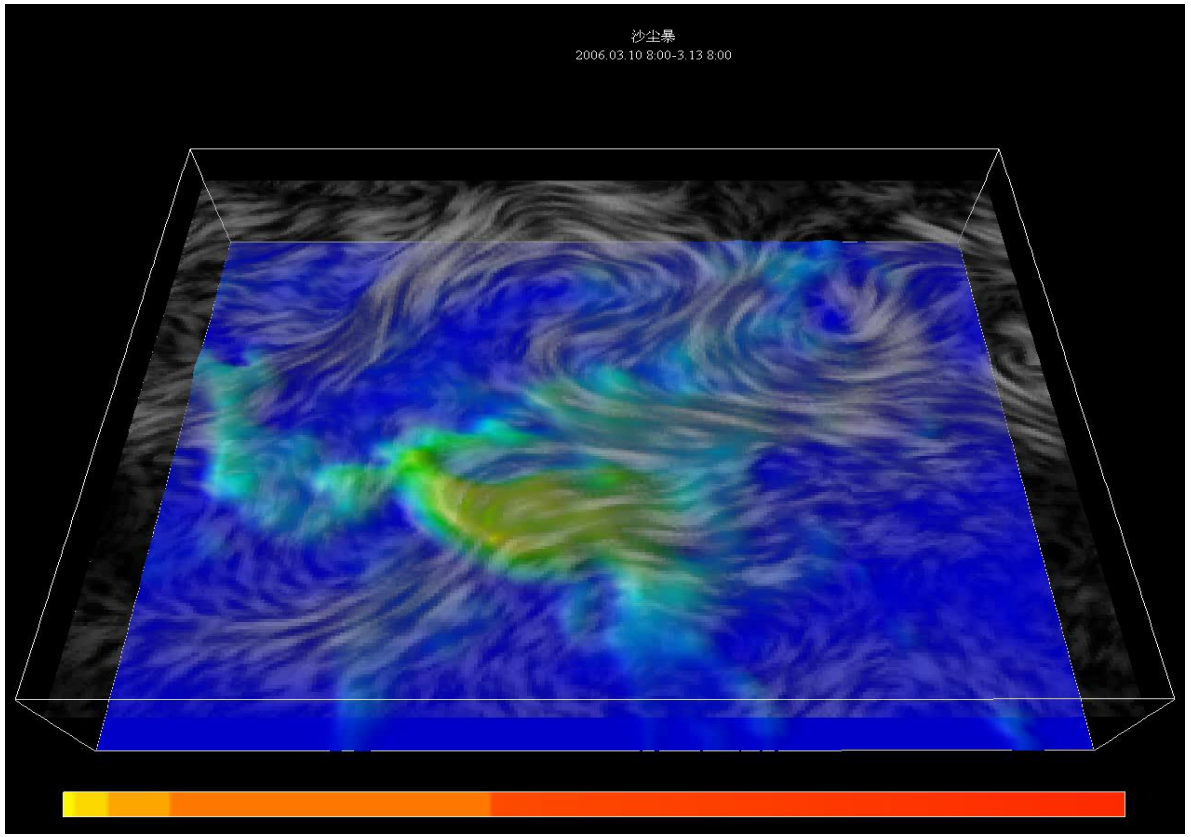
# Applications in Science and Engineering

1. Scientific Research
2. Industrial Computing

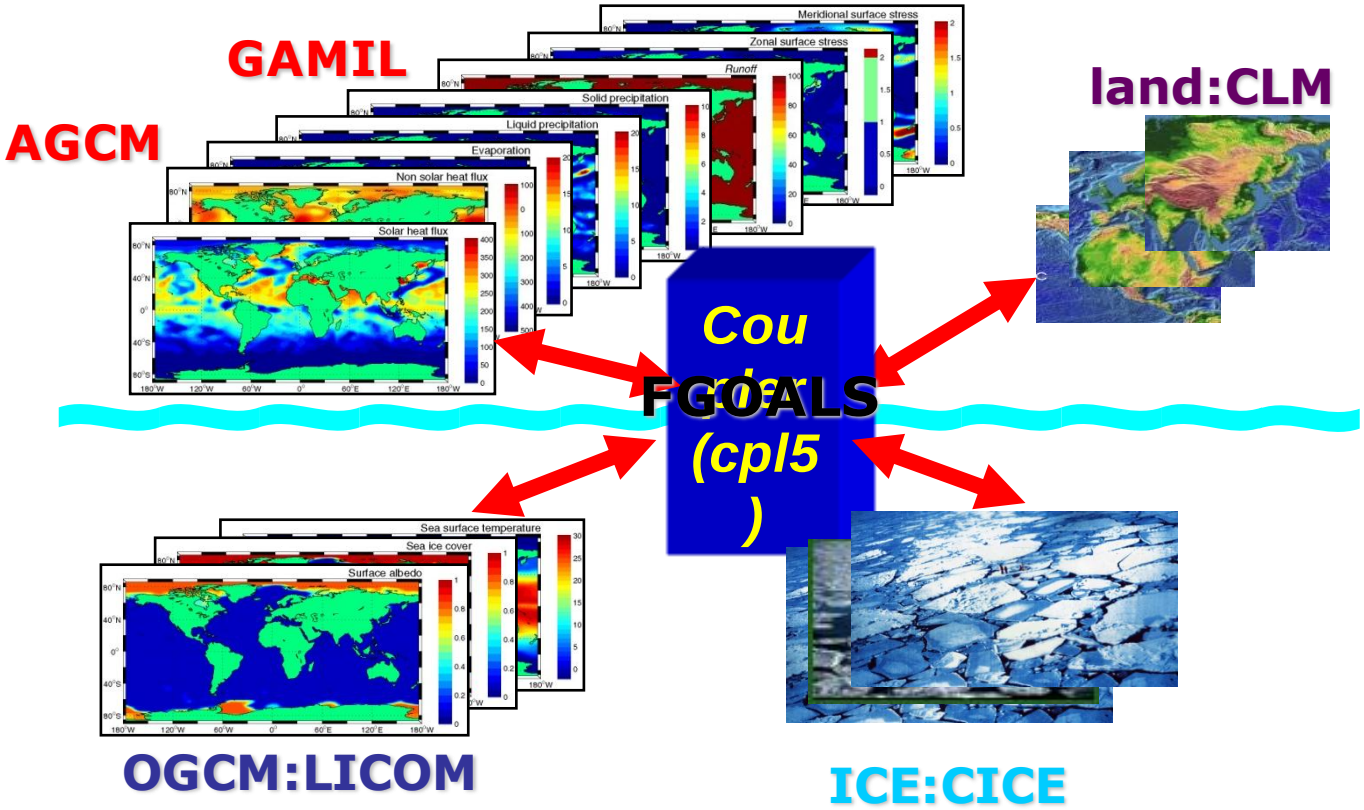
# Prediction of Sandstorm

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

  down to 8mins



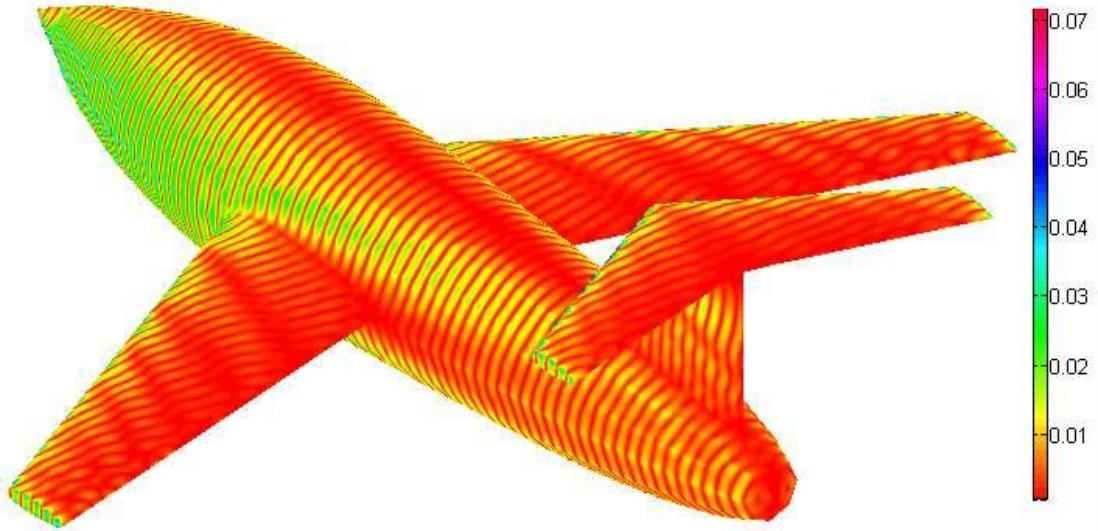
# Global Climate Model-FGOALS

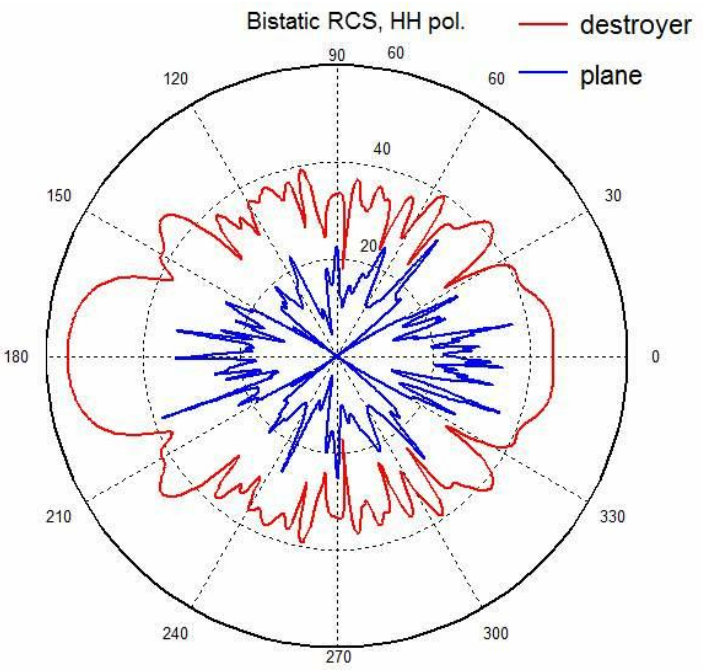


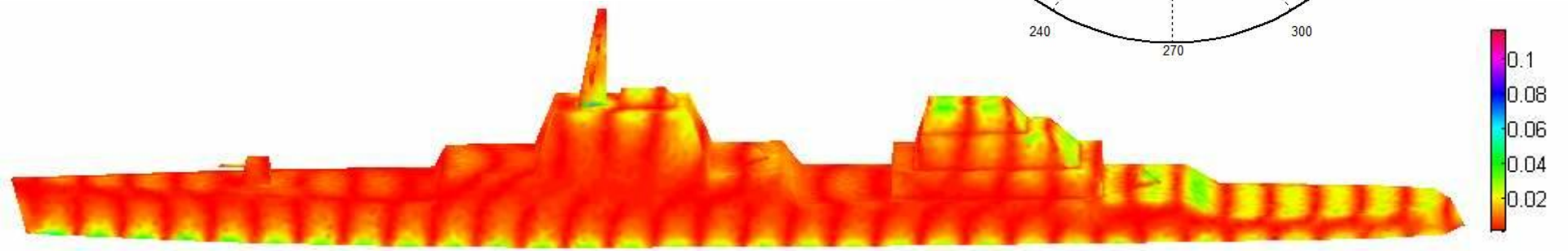

| CPU | AGCM | LAND | OGCM | ICE | Coupler |
|---|---|---|---|---|---|
| 1620 | 720 | 90 | 540 | 180 | 90 |

# EM Scattering

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



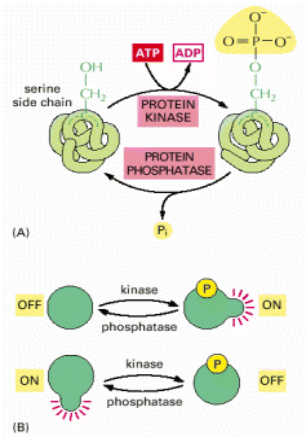



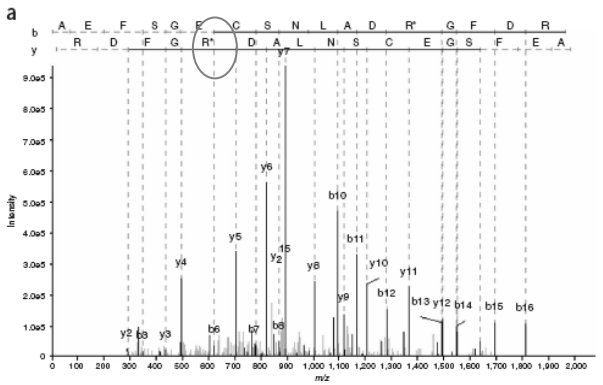



# P_InsPecT/cuda-InsPecT Software

## 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

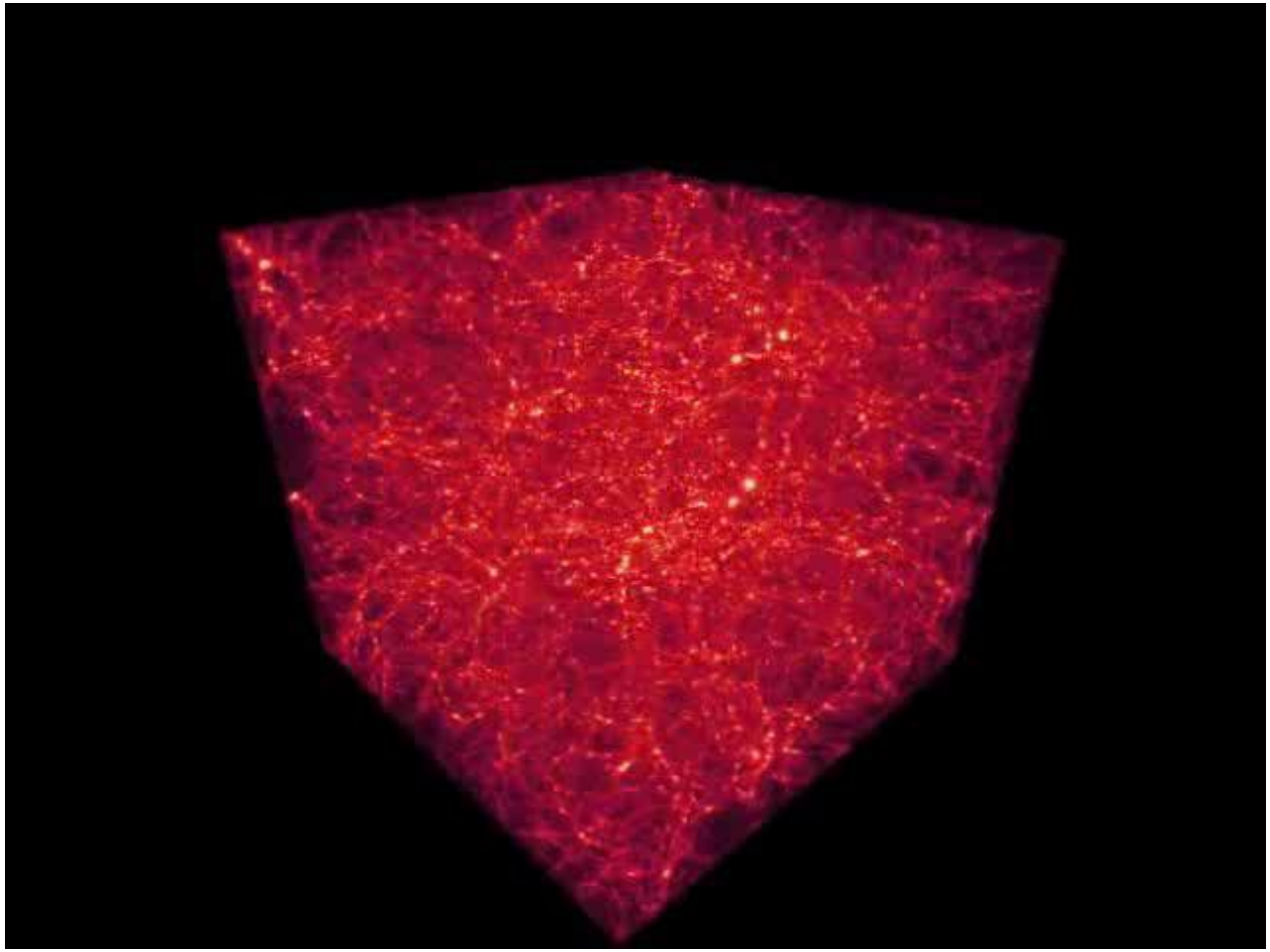
Software : P_InsPecT ( one modification )
Database : 36547 mass spectrometric;
107962 protein sequences
Environment : DeepComp7000

| | 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

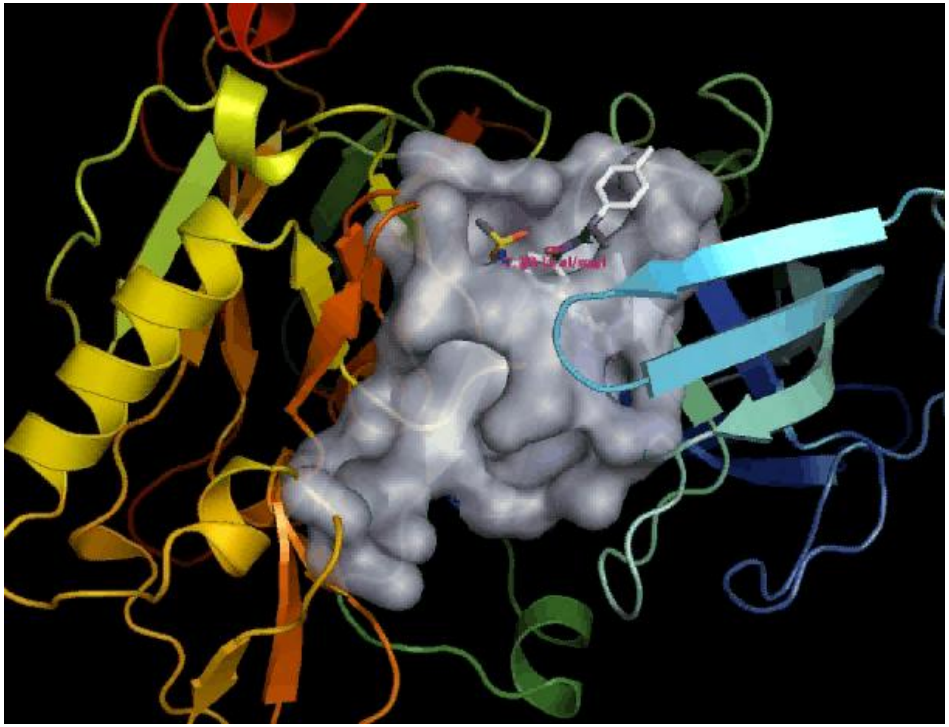
| | One Core ( estimate ) | 677 Fermi C2050 |
|---|---|---|
| Time | 6 years | 2.034 h |

# C4: Computational Cosmology Consortium of China



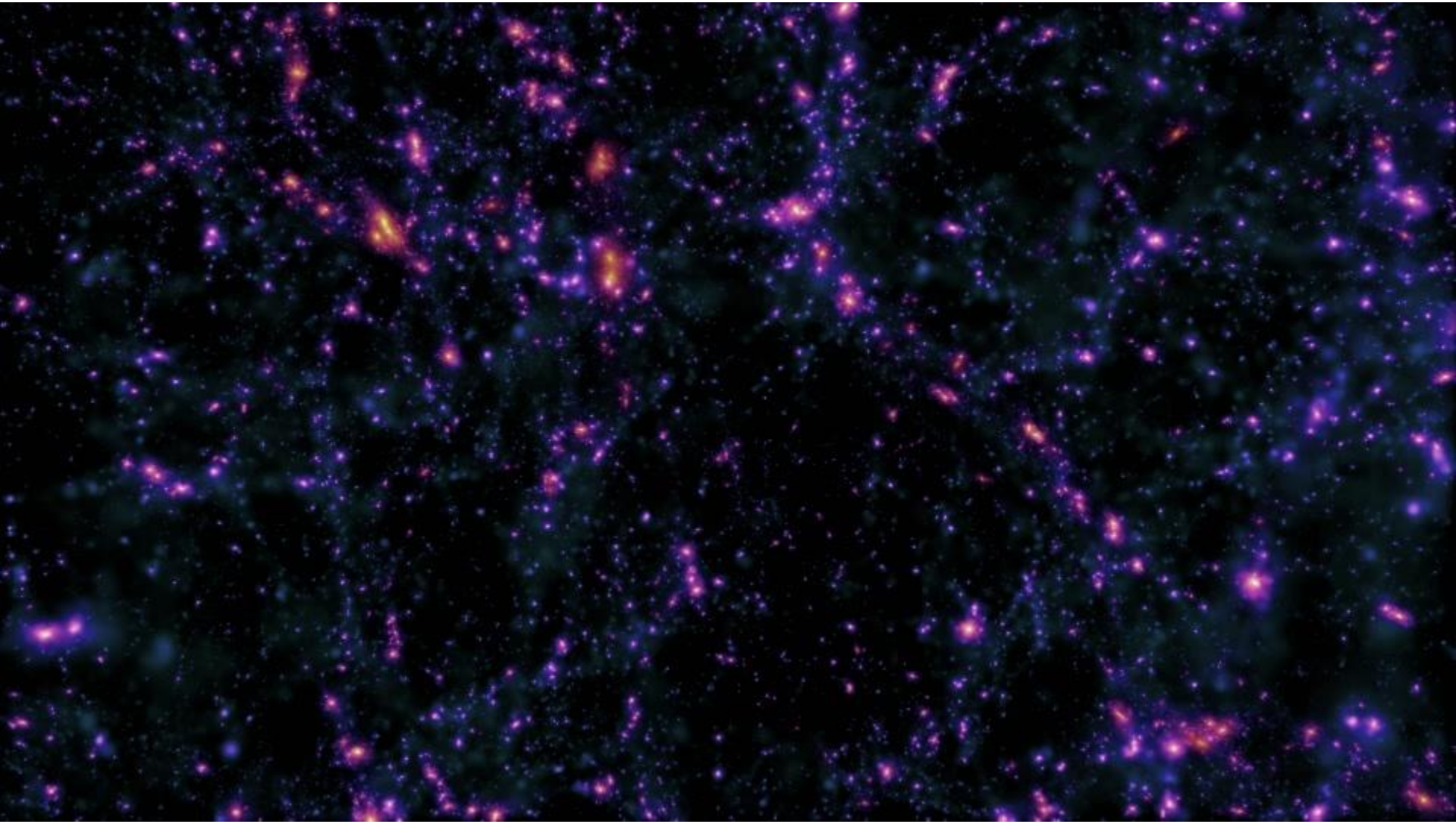
# Drug Screening for Curing Avian Influenza

- On DeepComp 7000
- 2400 CPU/cores were used
- Time: 2 months (128 CPU/cores) ⟶ 8 hours
- The compounds screened out by this simulation are in further biological test

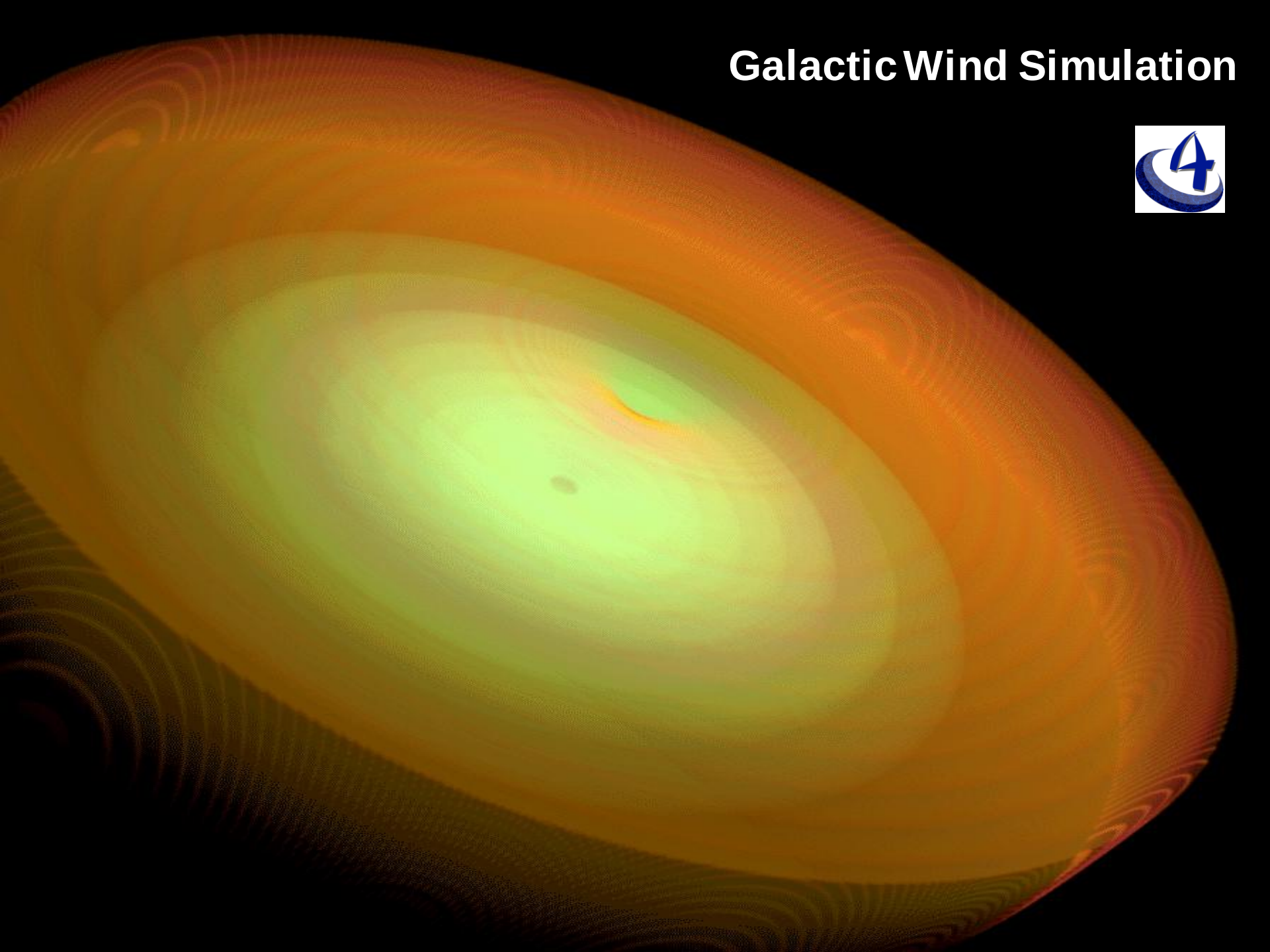


*Shanghai Institute of Materia Medica, Chinese Academy of Sciences

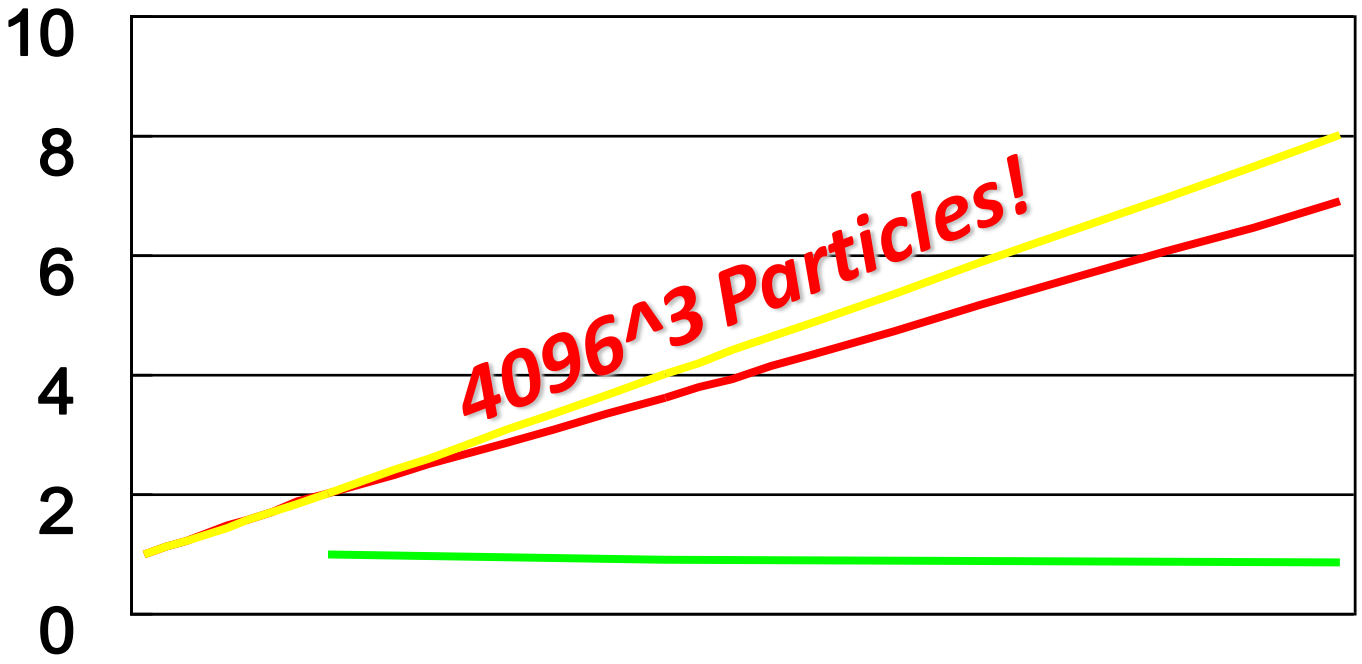
# Simulation of Universe Evolution



# Galactic Wind Simulation



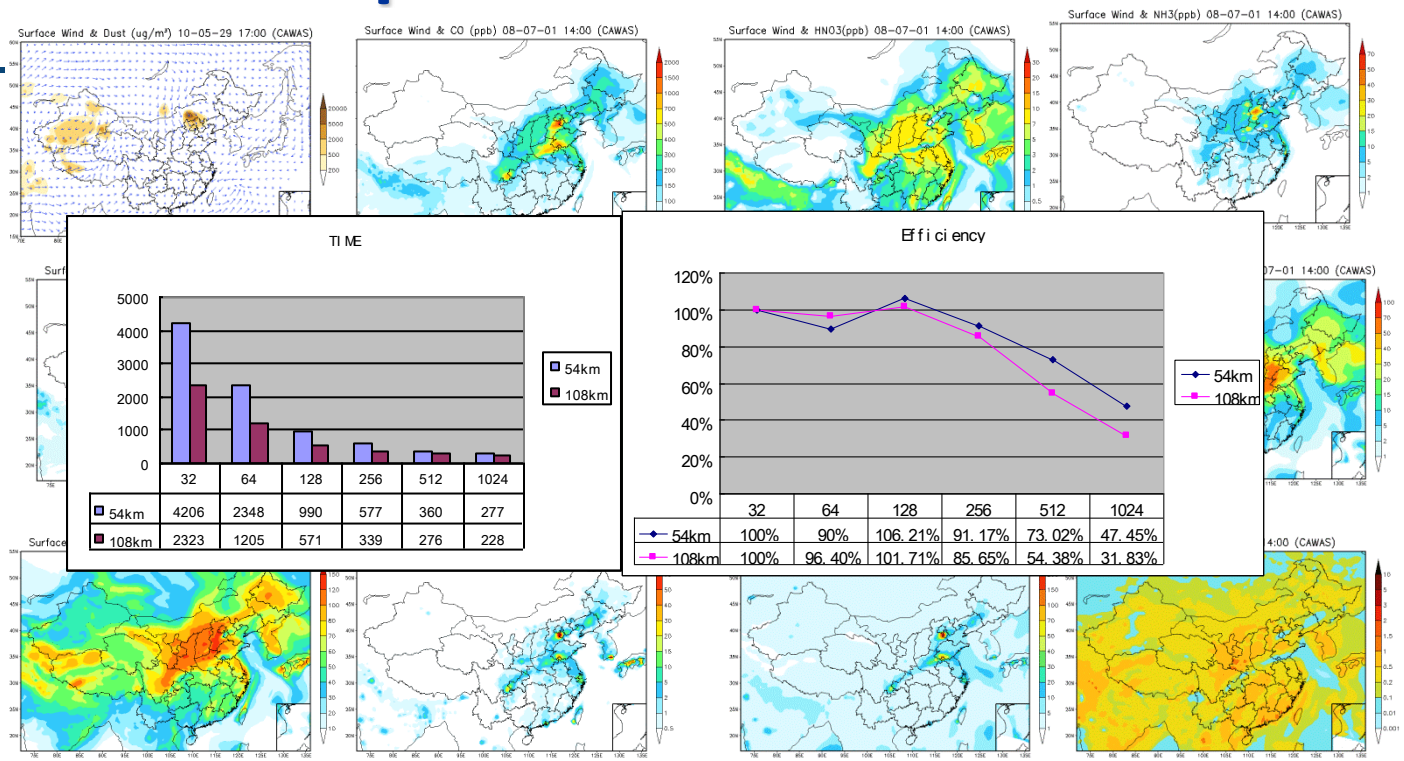
# Galactic Wind Simulation on Tianhe-1A



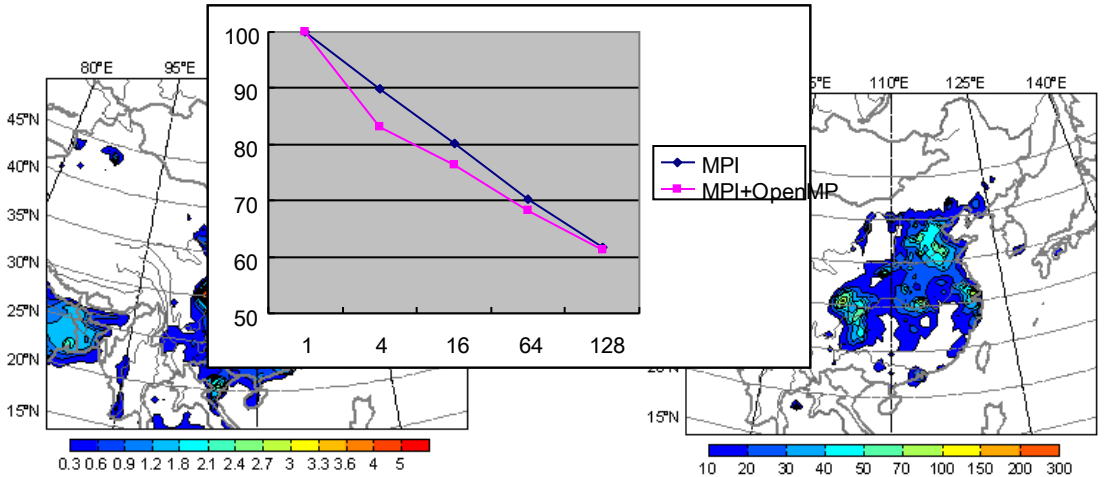

| | 2048 | 4096 | 8192 | 2E+04 |
|---|---|---|---|---|
| Speedup | 1 | 1. 996 | 3. 62 | 6. 9 |
| Li near | 1 | 2 | 4 | 8 |
| Ef f i ci ency | | 99. 79% | 90. 54% | 86. 20% |

# Climate and Atmosphere Model

**CUACE(CMA Unified Atmospheric Chemistry Environment)**




**RIEMS(*Regional* Integrated Environment Modeling System)**



# Simulation: Side-plates Formation in Ti-Alloys

**Phase-field model**

Time-dependent Ginzburg-Landau(TDGL) equation

Cahn-Hillard equation

Anisotropic interfacial energy

**Grid size**

1024*1024*1024

**Number of DOFs**

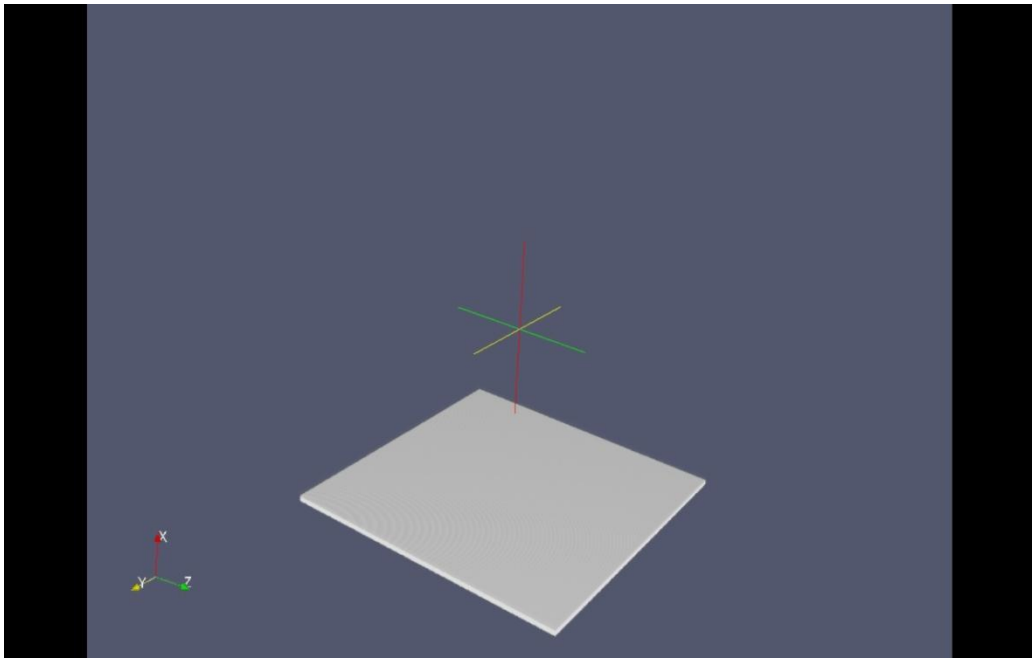
$4.295*10^9$

**Run on 4,096 cores**

Parallel efficiency 94%.

**Collaborators**

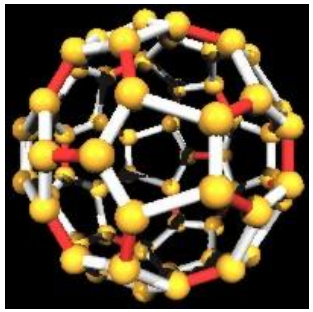
Ms. Mei Yang
Dr. Hao Wang
Dr. Gang Wang
Prof. Dongsheng Xu
Institute of Metal Research, CAS, Shenyang



**Side-plates Formation Visualization**

# Parallel Eigenvalue Solver — HPSEPS

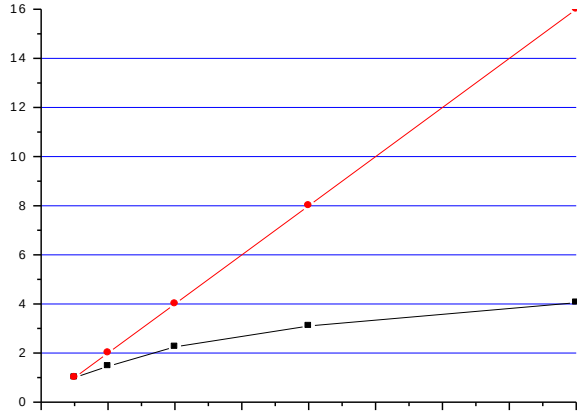
- Eigenvalue problem parallel solvers for sparse and dense symmetric matrix
- SVD Parallel Solver
- LSQR Parallel Solver



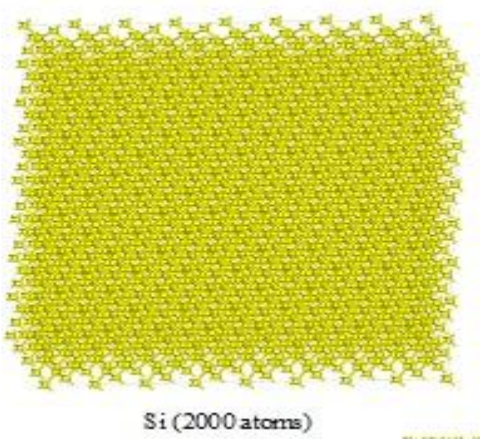
$$H\psi_i = E_i\psi_i \quad \Rightarrow \quad H(X)X = X\Lambda$$

| Num of cores | 512 | 1024 | 2048 | 4096 |
|---|---|---|---|---|
| Time(sec) | 2220.6 | 1350.4 | 912.5 | 662.6 |
| Parallel efficency | 100% | 82% | 61% | 42% |

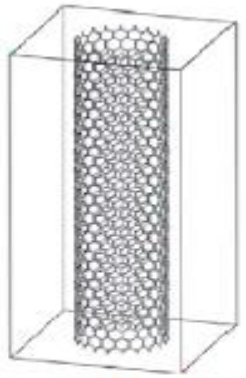
- Eigensolver for dense matrices with 8192 cores on Tianhe-1A ( N=40000 )




| Num of Cores | 512 | 1024 | 2048 | 4096 | 8192 |
|---|---|---|---|---|---|
| Time(sec) | 1058 | 723 | 471 | 341 | 261 |
| Speed up | 1.00 | 1.46 | 2.25 | 3.10 | 4.05 |
| Efficency | 100% | 73% | 56% | 39% | 25% |



Si (2000 atoms)

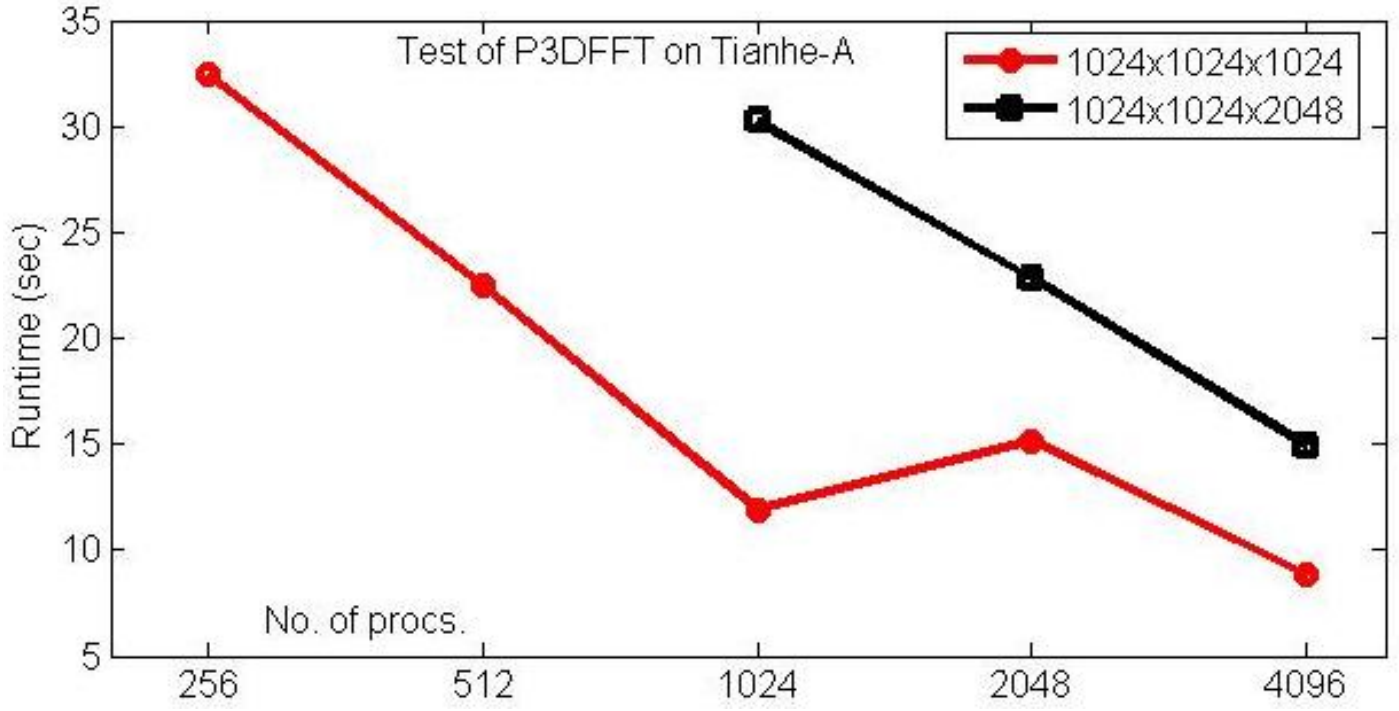


(21.37,0 ) Nano tube (1200 atoms)

# P3DFFT on Tianhe-1 A

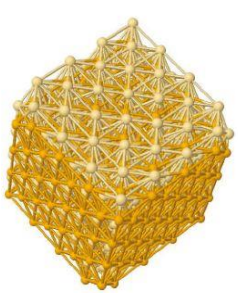
- **Parallel 3D FFT**
  - Based on FFTW3.2.1, but MPI_All to All is avoid

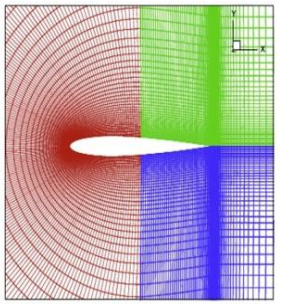
| | 1024x1024x1024 | | | | | 1024x1024x2048 | | |
|---|---|---|---|---|---|---|---|---|
| #Procs. | 256 | 512 | 1024 | 2048 | 4096 | 1024 | 2048 | 4096 |
| T(P3DFFT) | 32.42 | 22.44 | 11.91 | 15.17 | 8.83 | 30.26 | 22.79 | 14.95 |
| Efficiency | 1 | 0.72 | 0.68 | 0.26 | 0.23 | 1 | 0.66 | 0.51 |

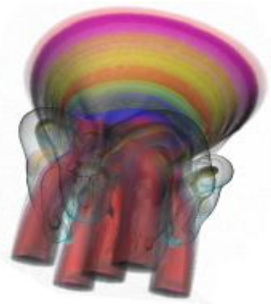


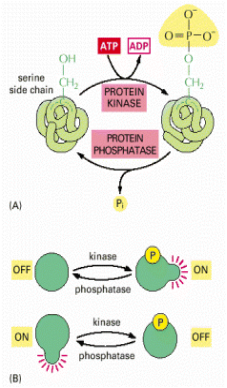
# GPU applications in SCCAS

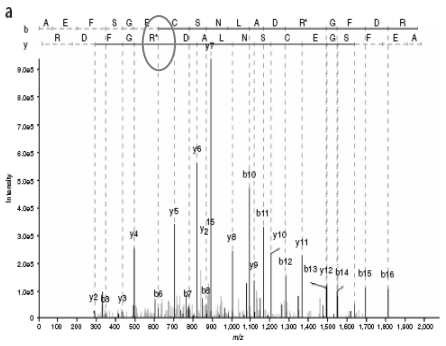
- **Accelerating scientific discovery using GPU technology:**
  - ✓ Computational bioinformatics
  - ✓ Material science
  - ✓ Seismic wave simulation
  - ✓ Visualization: volume rendering
  - ✓ Numerical computation: SVD
  - ✓ Graphics：Bucket Depth Peeling Mega Image Matting
- **CFD**
  - ✓ Cavity flow; 2D Riemann problem
  - ✓ Airfoil RAE2882; OpenCFD code

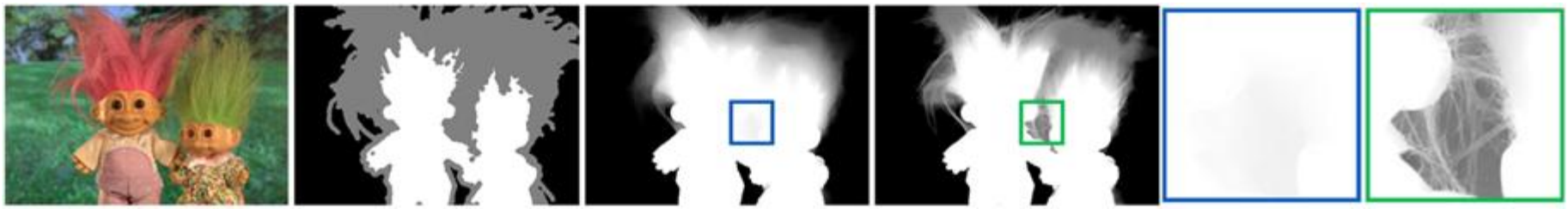






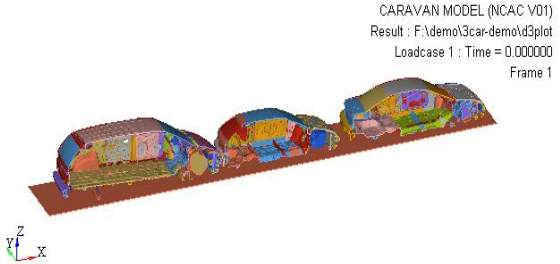




# CAD/CAE Platform in Automation Industry

- **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



# International Collaborations

- **NCSA/UIUC**
  - ACCESS
    - ✓ HPC(2009,Beijing), DISC(2010,Urbana-Champaign), Visualization (2011, Xi'an)
  - Fault-Tolerance
    - ✓ Marc Snir (NCSA/UIUC)
    - ✓ Franck Cappello (INRIA/UIUC)
  - Grid – interoperationality
    - ✓ John Towns (NCSA/UIUC)
- **Juelich, Germany**
- **Seeking for more**
  - France (GENCI, etc)
  - Japan (RIKEN, etc)


# Future Plan on High Performance Environment in CAS

# Petascale Supercomputers

- **1 PetaFlops computer in 2013**
  - Budget approximately 250M RMB
  - For scientific computing
- **X PetaFlops computer at the end of 12th five-year plan**
  - Collaboration with Beijing local government
  - Budget under discussion
  - For scientific computing and industry computing

# Question & Suggestion

# Thank you very much!