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Recent Advances of Chinese Efforts in HPC

Zhong Jin
Supercomputing Center
CNIC, CAS

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Current Status and Recent Advances

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Funding Agencies of HPC in China

- MOST – 863 Program (HW, SW & Apps)
- CAS – Informization Project (HW, SW & Apps)
- NSFC – General projects (Apps)
- Ministries funding (SW)
- Local government funding (HW)

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Roadmap of HPC in CAS

CAS - a pioneer of HPC and applications in China

SGI Power Challenge XL
6.4 GFlops

Hitachi SR2201
9.6 GFlops

Dawning-2000 II
110 GFlops

Lenovo DeepComp7000
145.97 TFlops

Lenovo DeepComp6800
5.3 TFlops

Peta Flops

10 PFlops

1996 1998 2000 2003 2008 2012 2015

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SCCAS' R&D in HPC

- **Parallel Algorithm**
  - ✓ **AMR (Adaptive Mesh Refinement)**
  - ✓ **Eigenvalue Problem - PSEPS**
  - ✓ **Fast Multipole Method**
  - ✓ **Computing Model**
- **Applications**
  - ✓ **Drug design**
  - ✓ **Astrophysics**
  - ✓ **Climate simulation**
  - ✓ **Material science**
  - ✓ **....**
- **ScGrid**
  - ✓ Middleware
  - ✓ Application
    - ➢ Gridmol – Computational Chemistry

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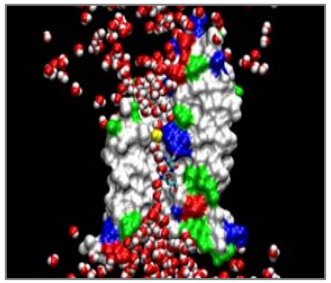
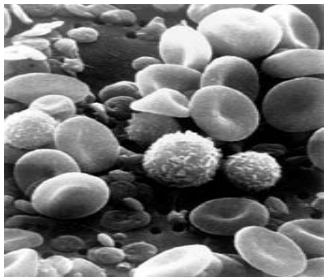
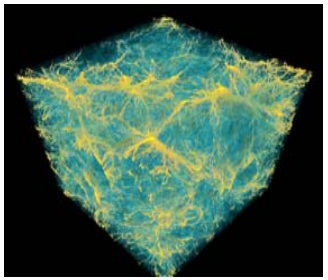
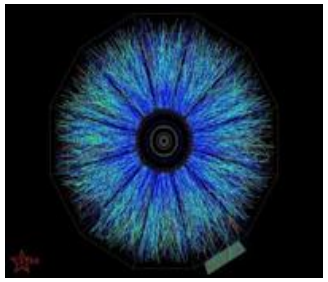
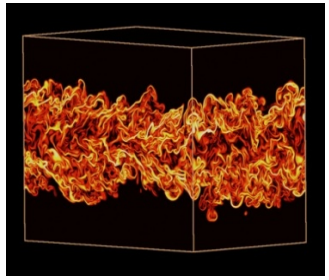
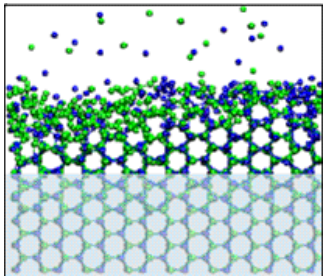
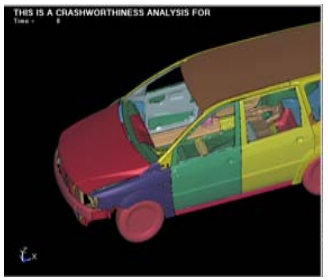
Projects toward large scale application

- **Objective**
  - ✓ Encourage application scientists to develop large scale applications and to use supercomputer more efficiently
- **Application fields**
  - ✓ Drug Design
  - ✓ Earth Science
  - ✓ Earthquake
  - ✓ Fluid Dynamics
  - ✓ Astrophysics
  - ✓ High Energy Physics
  - ✓ Oil Exploration
  - ✓ Imaging of SEM
  - ✓ Material Science
  - ✓ Nano Science





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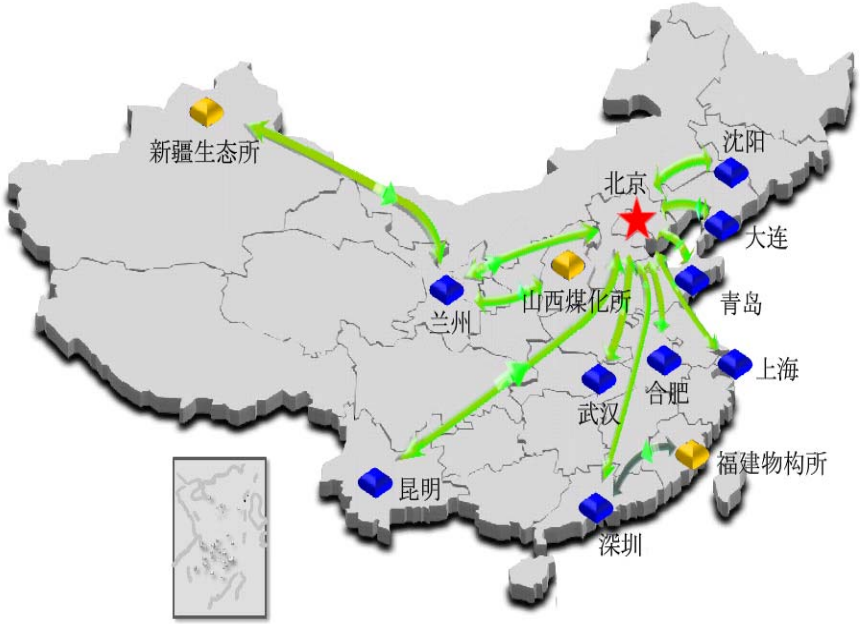
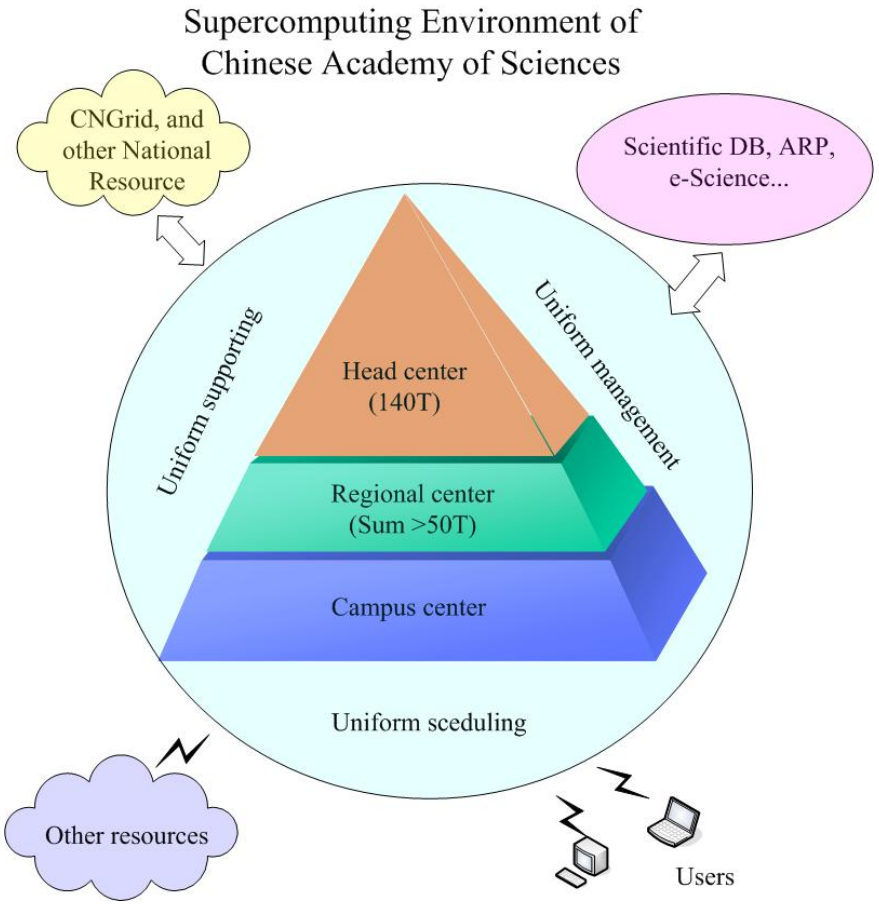
China Scientific Computing Grid (ScGrid)





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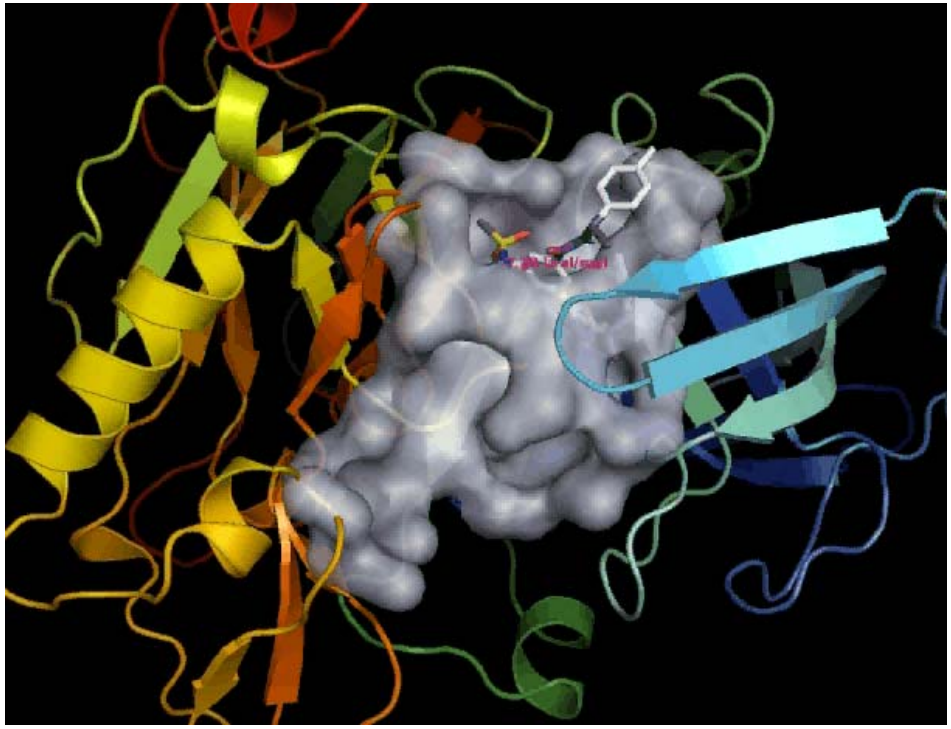
Drug Screening for Curing Avian Influenza

- **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

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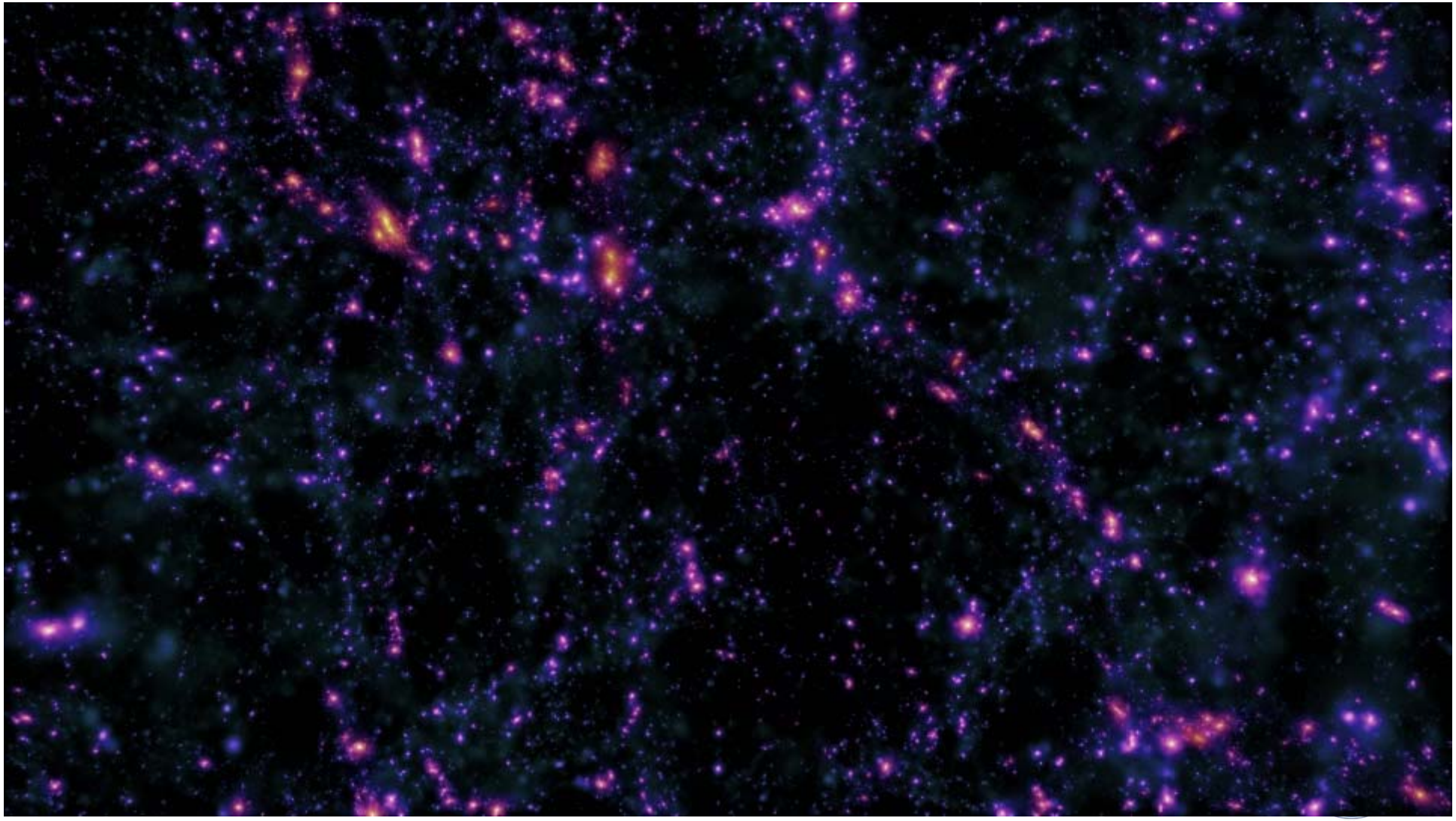
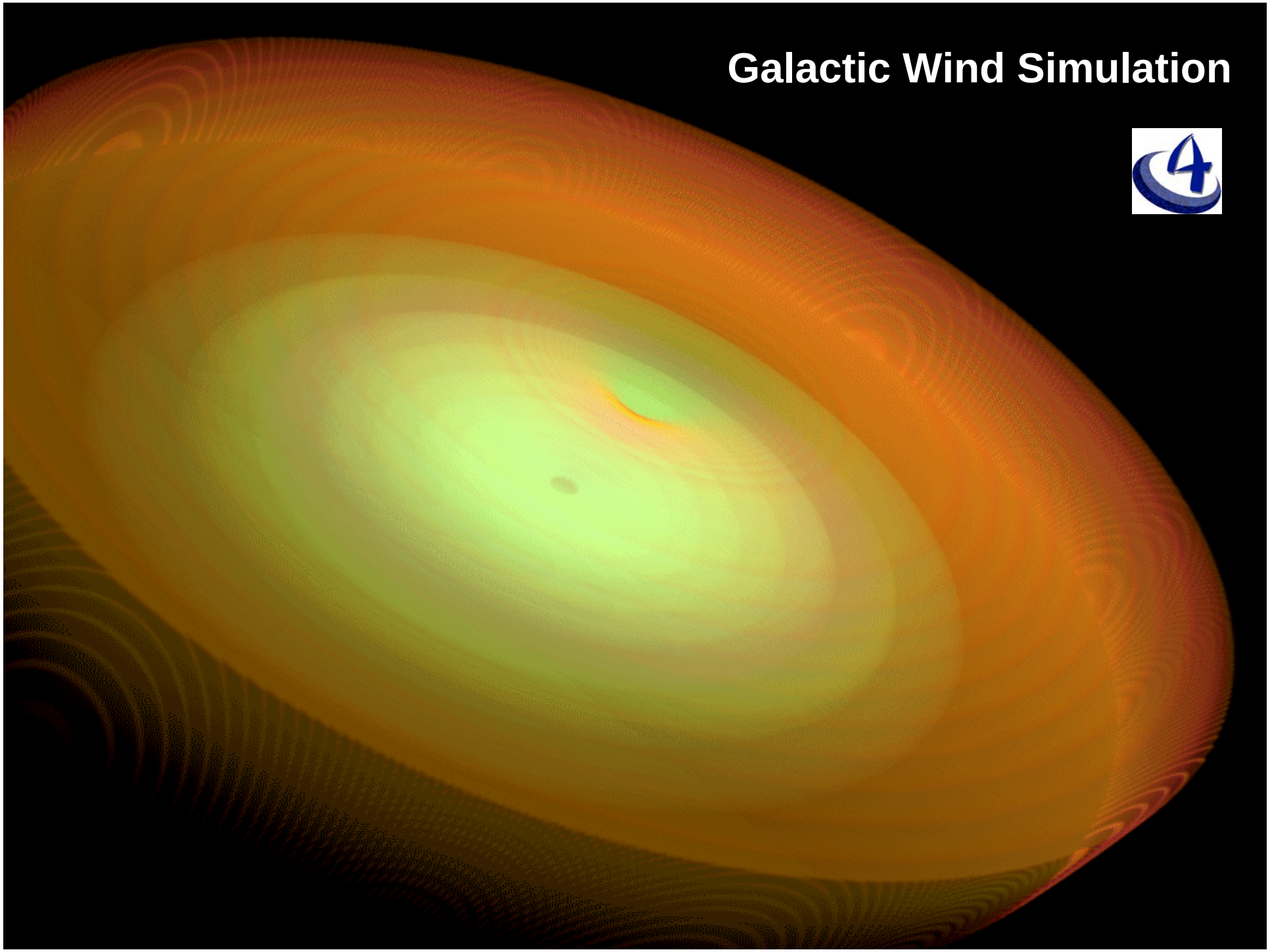
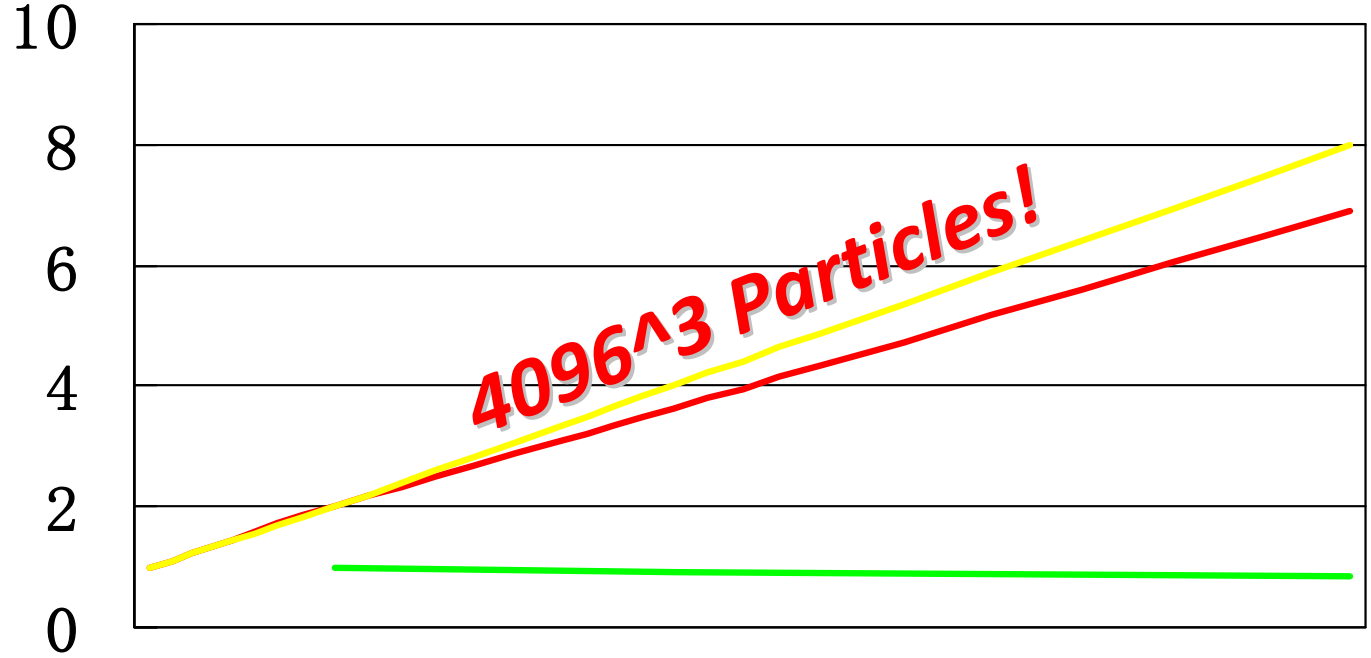
Simulation of Universe Evolution



Galactic Wind Simulation



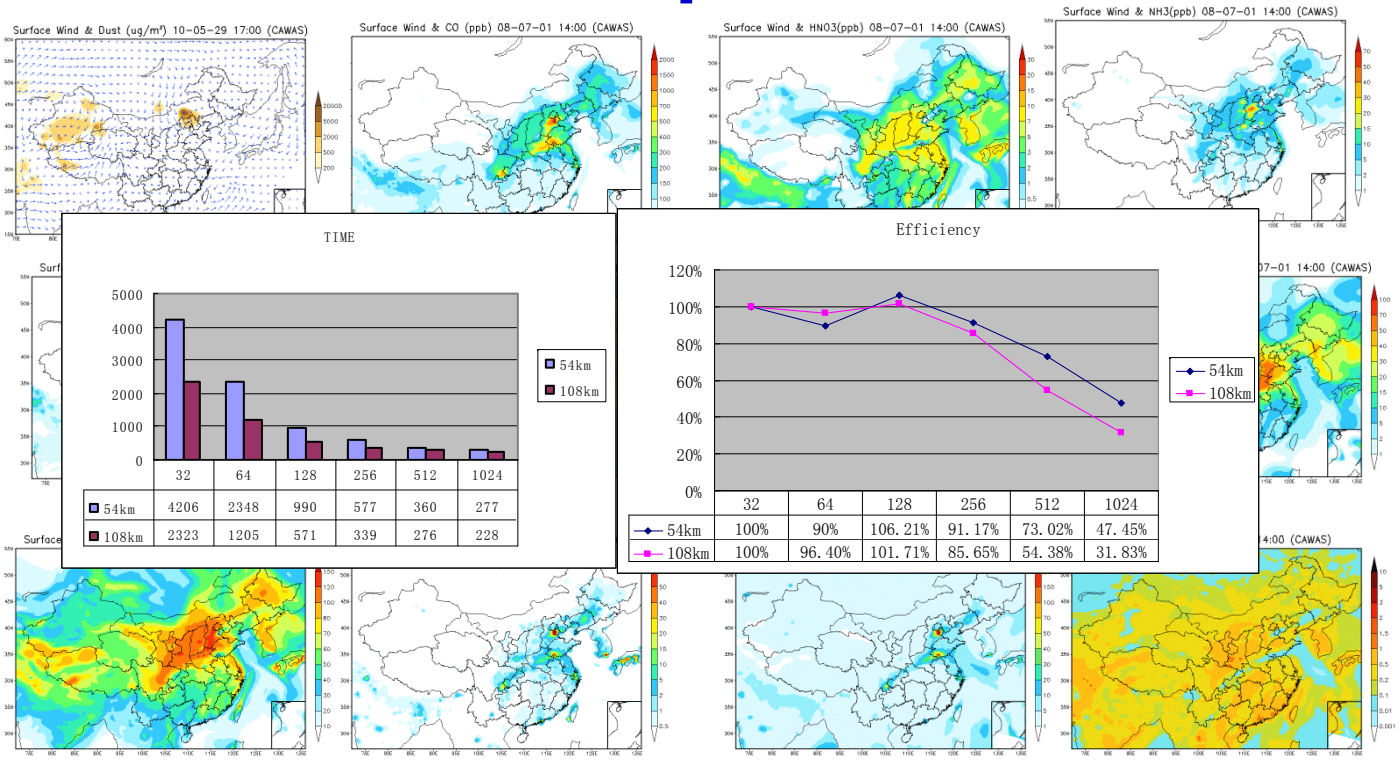
Galactic Wind Simulation on Tianhe-1A



	2048	4096	8192	16384
Speedup	1	1.996	3.62	6.9
Linear	1	2	4	8
Efficiency		99.79%	90.54%	86.20%

Climate and Atmosphere Model

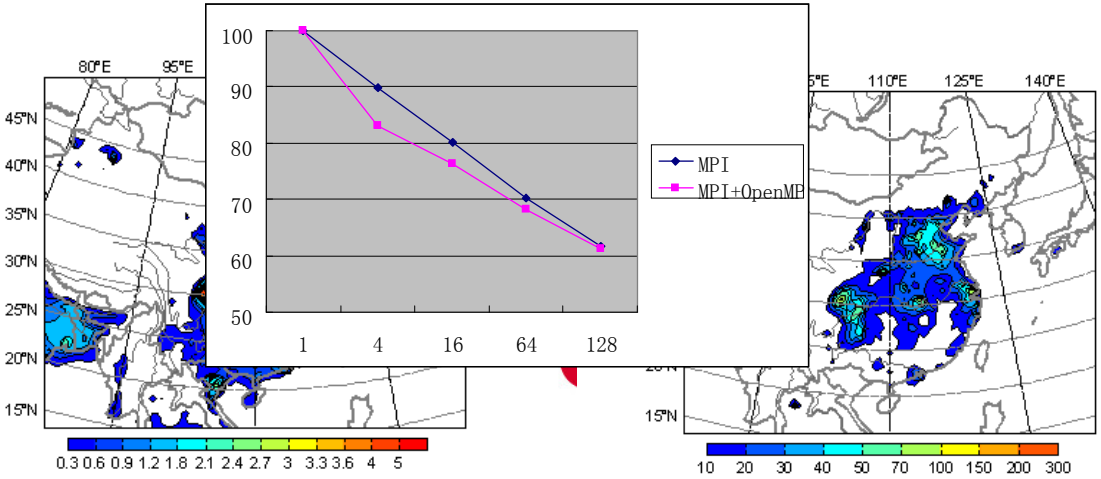
CUACE(CMA
Unified
Atmospheric
Chemistry
Environment)



	32	64	128	256	512	1024
54km	4206	2348	990	577	360	277
108km	2323	1205	571	339	276	228

	32	64	128	256	512	1024
54km	100%	90%	106.21%	91.17%	73.02%	47.45%
108km	100%	96.40%	101.71%	85.65%	54.38%	31.83%

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

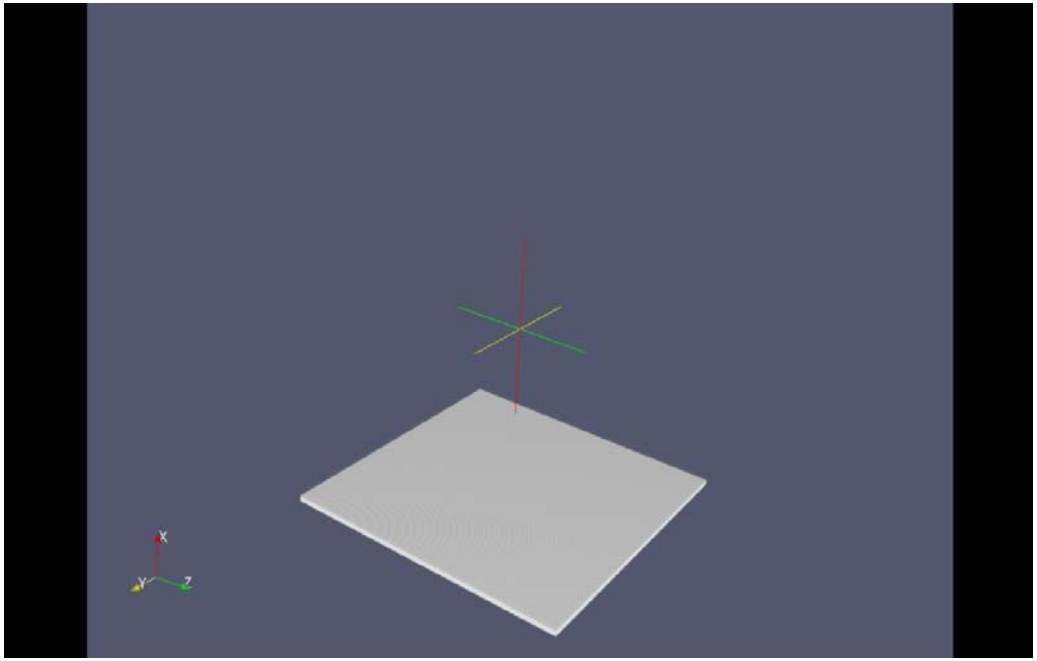
$4.295*10^9$

Run on 4,096 cores

Parallel efficiency 94%.

Collaborators

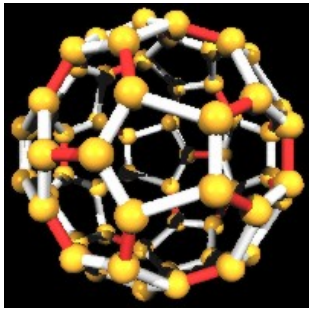
Ms. Mei Yang
Dr. Hao Wang
Dr. Gang Wang
Prof. Dongsheng Xu
Institute of Metal Research, CAS, Shenyang



Side-plates Formation Visualization

Parallel Eigenvalue Solver — HPSEPS

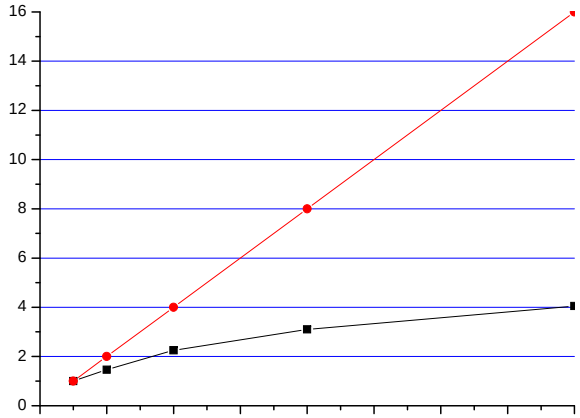
- Eigenvalue problem parallel solvers for sparse and dense symmetric matrix
- SVD Parallel Solver
- LSQR Parallel Solver



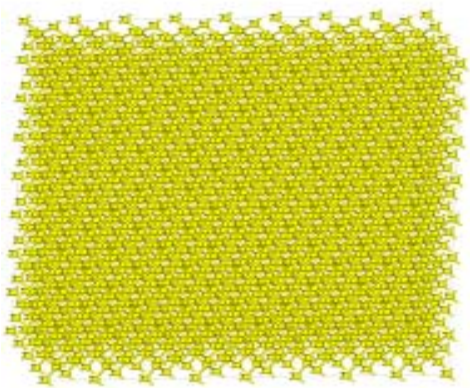
$$H\psi_i = E_i\psi_i \rightarrow H(X)X = X\Lambda$$

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

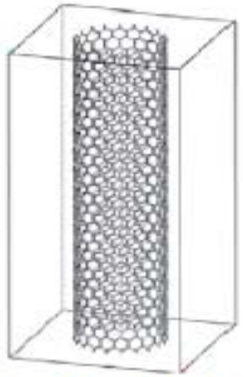
- **Eigensolver for dense matrices with 8192 cores on Tianhe-1A（N=40000）**



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)

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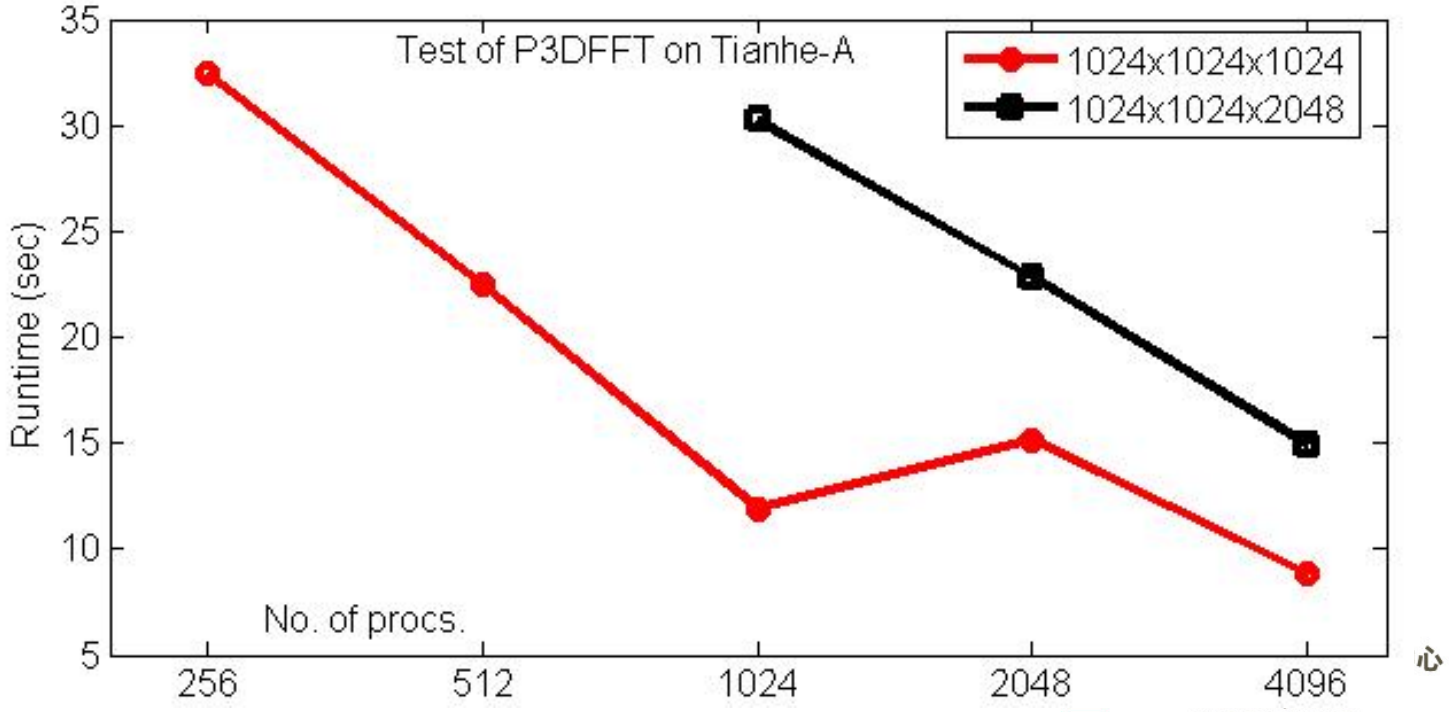
P3DFFT on Tianhe-1 A

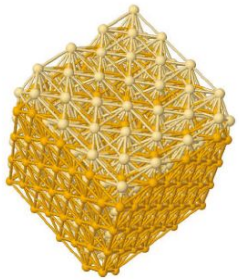
- **Parallel 3D FFT**
  - Based on FFTW3.2.1, but MPI_All to All is avoid

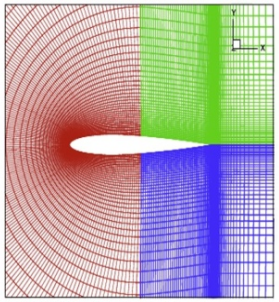
	1024x1024x1024					1024x1024x2048		
#Procs.	256	512	1024	2048	4096	1024	2048	4096
T(P3DFFT)	32.42	22.44	11.91	15.17	8.83	30.26	22.79	14.95
Efficiency	1	0.72	0.68	0.26	0.23	1	0.66	0.51

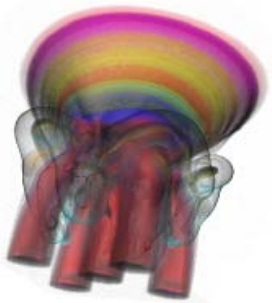


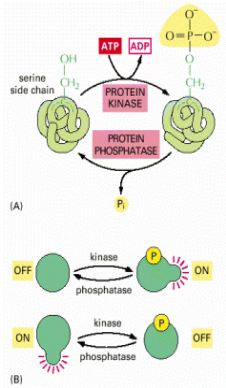
GPU applications in SCCAS

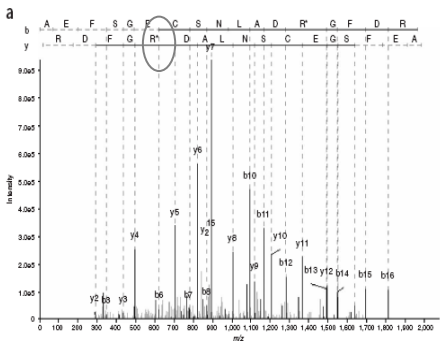
- **Accelerating scientific discovery using GPU technology:**
  - ✓ Computational bioinformatics
  - ✓ Material science
  - ✓ Seismic Wave Simulation
  - ✓ Visualization: volume rendering
  - ✓ Numerical computation: SVD
  - ✓ Graphics：Bucket Depth Peeling Mega Image Matting
- **CFD**
  - ✓ Cavity flow;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

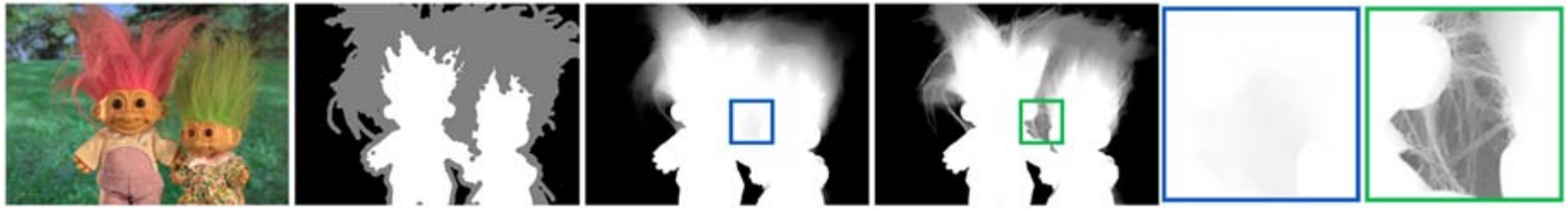












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International Collaborations

- **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)**

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863 Program on HPC and Grid

- **11th Five-year Plan (FY2006-FY2010)**
  - ✓ **High Productivity Computer and Grid Service Environment**
  - ✓ **740 millions CNY from the MOST + more joint investments from other sources**
  - ✓ **Major Activities**
    - ➢ **HPC HW**
    - ➢ **Grid Middleware**
    - ➢ **Operation of CNGrid**
    - ➢ **Applications**

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- **Phase I - Tera Era**
  - ✓ Lenovo DeepComp 7000 – SCCAS (Beijing)
    - ➢ Hybrid cluster
    - ➢ 145.97 TFlops (Peak)
    - ➢ 12320 CPU/Cores
    - ➢ 66 Terabytes memory

  - ✓ Dawning 5000A – SSC (Shanghai)
    - ➢ Low power CPU & high density blades
    - ➢ 233.472 TFlops (Peak)
    - ➢ 30720 CPU/Cores
    - ➢ 122.88 Terabytes memory

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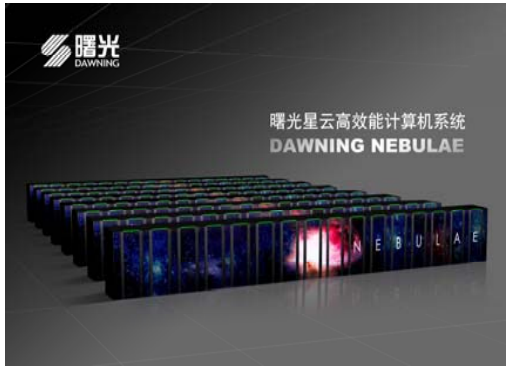
- **Phase II – Peta Era**
  - ✓ Tianhe-1A - Tianjin Supercomputing Center
    - A Hybrid system by NUDT
    - 2.566 PetaFlops (Linpack)
    - 186368 CPU/Cores
    - NUDT TH MPP, X5670 2.93Ghz 6C, NVIDIA GPU, FT-1000 8C

  - ✓ Nebulae - South China Supercomputing Center (Shenzhen)
    - A hybrid system by Dawning
    - 1.271 PetaFlops (Linpack)
    - 120640 CPU/Cores
    - Dawning TC3600 Blade, Intel X5650, NVidia Tesla C2050 GPU



  - ✓ Shandong Supercomputing Center (Jinan)
    - Will be coming soon

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China National Grid (CNGrid)

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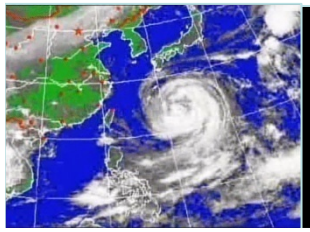
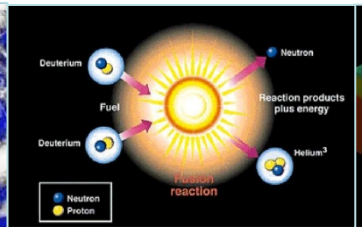
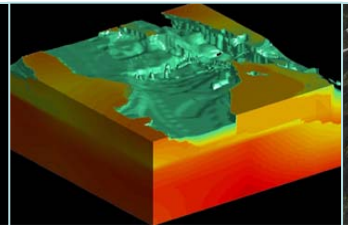
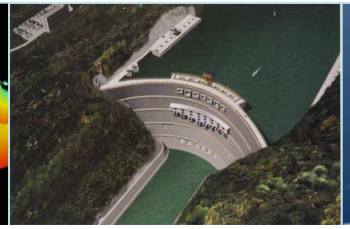
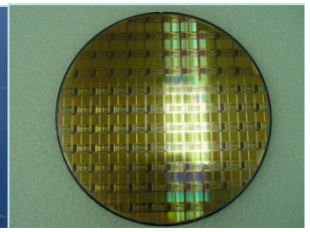
Grid and HPC Applications

- Developing productive HPC and Grid applications
- Verification of the technologies
- Applications from some selected areas
  - ✓ Resource and Environment
  - ✓ Research
  - ✓ Services
  - ✓ Manufacturing



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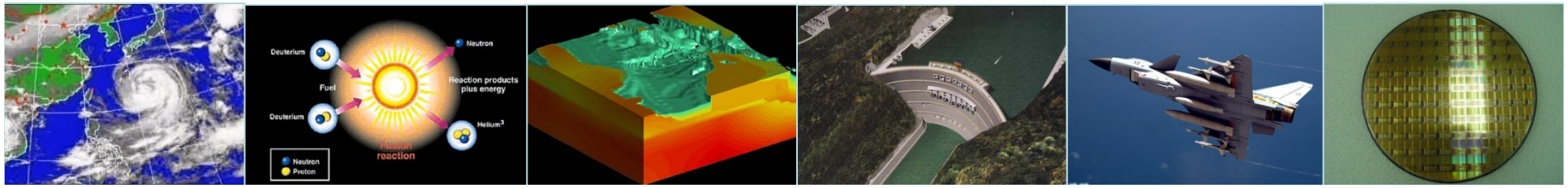
HPC applications

- Computational chemistry
- Computational Astronomy
- Parallel program for large fluid machinery design
- Fusion ignition simulation
- Parallel algorithms for bio- and pharmacy applications
- Parallel algorithms for weather forecasting based on GRAPES
- 10000+ core scale simulation for aircraft design
- Seismic imaging for oil exploration
- Parallel algorithm libraries for PetaFlops systems



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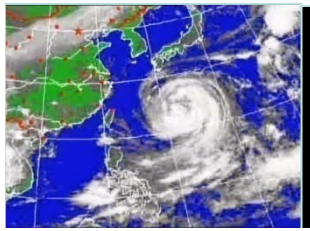
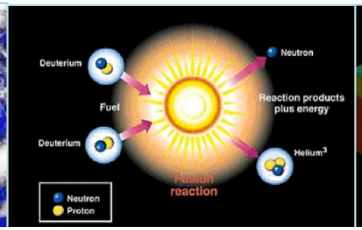
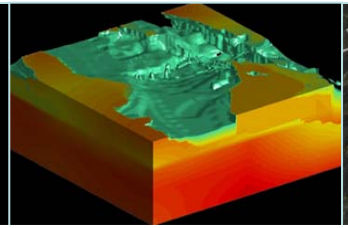
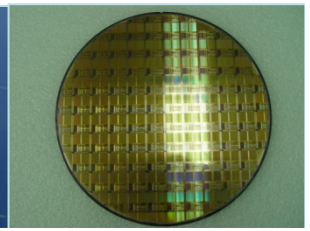
Grid applications

- Drug Discovery
- Weather forecast
- Scientific data grid and its application in research
- Water resource information system
- Grid-enabled railway freight information system
- Grid for Chinese medicine database applications
- HPC and Grid for Aerospace industry (AviGrid)
- National forestry project planning, monitoring and evaluation



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Future Plan

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Petascale Supercomputers and Applications in CAS

- **2012 - PetaFlops computer and applications**
  - ✓ Budget: CNY 250 Millions
  - ✓ Toward scientific computing
  - ✓ New facility and campus will be constructed in the suburb of Beijing
  - ✓ Research center of specific application is required
- **2015 - 10 PetaFlops computer**
  - ✓ Collaborating with Beijing local government
  - ✓ Budget: CNY 700 Millions
  - ✓ Toward scientific computing and industry computing

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Era of Petascale and beyond in China

- **12th Five-year Plan (2011-2015)**
  - ✓ **Several petascale HPCs**
  - ✓ **At least one 50-100 PFLOPS HPC**
  - ✓ **Budget: CNY 4 Billions**
    - ➢ **MOST: 60%**
    - ➢ **Local Government: 40%**
- **13th Five-year Plan (2016-2020)**
  - ✓ **1~10 ExaFLOPS HPC**
  - ✓ **Budget: unknown yet**

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Thank you!

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